67th ASMBLY TFS

Welcome to the 67th ASMS Conference on Mass Spectrometry and Allied Topics. Conference program activities and exhibit booths are in the Georgia World Congress Center. Corporate Member hospitality suites are located in the Omni CNN Hotel.

SPONSORS

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PROGRAM HIGHLIGHTS

REGISTRATION, is open 10:00 am - 8:00 pm on Sunday and 7:30 am - 5:00 pm Monday - Thursday, Building B Main Lobby

ATTENTION UNDERGRADUATE STUDENTS AND FIRST TIME (AT ASMS) GRADUATE STUDENTS
4:00 - 4:45 pm, Sunday, B302-305, Level Three
Plan Your Strategy: What to See and Do at ASMS

TUTORIALS

SUNDAY TUTORIAL SESSION I, 5:00 - 6:30 PM
Murphy Ballroom, Level Five





5:00 - 5:45 pm
Lipidomics

Stephen Blanksby
Queensland Univ. of Technology
& Gavin Reid
University of Melbourne



5:45 - 6:30 pm
Targeted Imaging

Enrico Davoli
Mario Negri Institute

SUNDAY TUTORIAL SESSION II, 5:00 - 6:30 PM
B302-305, Level Three



5:00 - 5:45 pm
Native Mass Spectrometry

Michal Sharon
Weizmann Institute



5:45 - 6:30 pm
Data Independent Acquisition

Birgit Schilliing
The Buck Institute

PLENARY SESSIONS

SUNDAY CONFERENCE OPENING, 6:45 - 7:45 PM
Murphy Ballroom, Level Five



Welcome

Susan Richardson
University of South Carolina
ASMS Vice President for Programs



Transitioning the World Energy for All Purposes to Stable Electricity Powered by 100% Wind, Water, and Sunlight

Mark Z. Jacobson
Stanford University

SUNDAY WELCOME RECEPTION, 7:45 - 9:00 PM
Poster/Exhibit Hall, Hall B-2 & B-3, Level One.
Conference name badge is required.

MONDAY AWARD LECTURE, 4:45 - 5:30 PM
Murphy Ballroom, Level Five



John B. Fenn Award for a Distinguished Contribution in Mass Spectrometry

John R. Yates
The Scripps Research Institute

TUESDAY AWARD LECTURE, 4:45 - 5:30 PM
Murphy Ballroom, Level Five



Biemann Medal

Sarah Trimpin
Wayne State University

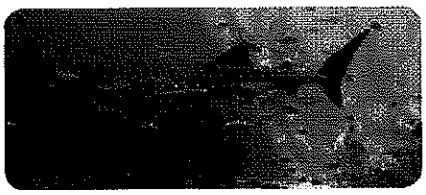
THURSDAY PLENARY SESSION, 4:45 - 5:30 PM
Murphy Ballroom, Level Five



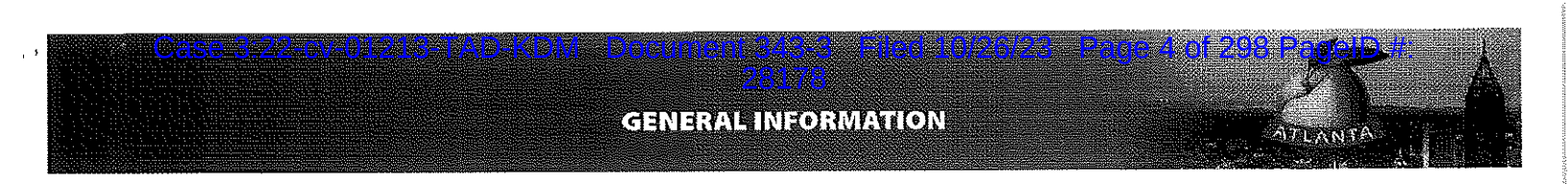
Chemistry of Food and Soft Drinks

Lilly D'Angelo
Global Food & Beverage Technology Associates

THURSDAY CLOSING EVENT AT THE GEORGIA AQUARIUM, 6:30 - 9:30 PM, $40/PERSON



Tickets must be purchased in advance by Monday 12 noon. Join us for an enchanting evening at the Georgia Aquarium. Dinner buffets close at 8:00 pm, dessert available until close. Ticket includes aquarium entry for our private event, dinner buffet and one drink ticket for soda, beer, or wine. Cash bars available until close



GENERAL INFORMATION

Oral Sessions are 8:30 - 10:30 am and 2:30 - 4:30 pm Monday through Thursday.

Building B – Level Five
Session A (MOA, TOA, WOA, ThOA)..... Murphy Ballroom
Building B – Level Four
Session B (MOB, TOB, WOB, ThOB) B401-402
Session C (MOC, TOC, WOC, ThOC) B405-407
Building B – Level Three
Session D (MOD, TOD, WOD, ThOD) B302-305
Session E (MOE, TOE, WOE, ThOE) B308-309
Session F (MOF, TOF, WOF, ThOF)..... B312-314
Building A – Level Four
Session G (MOG, TOG, WOG, ThOG) ..... Auditorium
Session H (MOH, TOH, WOH, ThOH) A411-412

Oral Presentations are projected from ASMS computers running Microsoft Office. Speakers are required to use the ASMS computers for their presentations.

Speakers must load presentations at least one day prior to their talks. The speaker ready room is B301, Building B, Level Three. The room is open with a technician according to this schedule:

Sunday: 10:00 am - 8:00 pm
Monday through Thursday: 7:30 am - 2:00 pm

Posters and Exhibit Booths are in the Poster/Exhibit Hall. The Hall is open:

Sunday Welcome Reception....7:45 pm - 9:00 pm
Monday - Wednesday .....7:00 am - 8:00 pm
Thursday .....7:00 am - 2:30 pm

Poster Set-Up is 7:00 - 8:00 am on the day scheduled. **Refer to the poster numbers in this final program for board assignments.** A counter for poster supplies is near the main entrance to the Hall.

History Posters are on display all week in Building B, Main Lobby.

Poster Sessions are 10:30 am - 2:30 pm, Monday through Thursday.

Poster Authors must be present at posters on scheduled days at these times. The following was new in 2018 (and may be new to some presenters for 2019) and allows for a one-hour non-overlapping lunch break. All presenters are now scheduled for 3 hours (authors welcome to attend the full four hours).

Odd-number posters present:
10:30 - 11:30 am PLUS 12:30 - 2:30 pm

Even-number posters present:
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Poster Pick-Me-Up Snacks served at 1:30 pm.

Presenters who must leave a poster unattended should post a return time. Presenters should wear "Poster Presenter" badges which are available at the poster supply counter.

Posters should be removed between 7:00 - 8:00 pm on Monday, Tuesday and Wednesday. Thursday posters should be removed between 2:30 - 3:00 pm.

Lunch Concessions in the Poster/Exhibit hall offer a variety of options to dine and network while taking a break from posters. Concessions are open 11:00 am - 2:00 pm, Monday through Thursday.

Exhibitors must staff exhibit booths as follows:
Sunday Reception ..... 7:45 pm - 9:00 pm
Monday - Thursday ..... 10:30 am - 2:30 pm

Workshops are 5:45 - 7:00 pm on Monday, Tuesday, and Wednesday. Light refreshments are provided on Level Three of Building A.

Dinner Break 7:00 - 8:00 pm is time for a breath of fresh air before the opening of hospitality suites at 8:00 pm.

Special Program for Undergraduate Students

- **Sunday, 7:30 - 9:00 pm, Poster competition**, Poster/ Exhibit Hall
- **Monday, 11:30 am - 1:00 pm, Meet the Experts.** Lunch tables reserved for undergraduate students in the Poster/ Exhibit Hall. Free vouchers for lunch will be provided at the tables. Arrive promptly at 11:30 am to obtain your voucher.

Free Wifi Access and Internet Stations are available throughout the convention center.

Conference Proceedings will be published online. Submission to the proceedings does not constitute publication and does not jeopardize the rights of authors to publish contents of their submissions. **Speaker slides will be printed to PDF and used as proceedings submission for speakers who fail to submit on their own.**

Webcasting includes tutorial lectures, plenary lectures, and oral sessions. Webcasts will be available to conference attendees for four months after the conference. ASMS does not retain rights to material included in webcasts.

Corporate Hospitality Suites may open 8:00 – 11:00 pm, Monday through Wednesday. Suites are located in the **Omni CNN Hotel.**

Career Center is located in B211-212. The Career Center is open to all conference attendees. Applicants and employers must enter resumes and employment opportunities online. There are computers in the center for searching the database of candidates and positions. Interview booths are available for onsite reservations (one-day advance reservation is recommended.)

Sunday .....7:45 - 9:00 pm
Monday - Wednesday .....7:30 am - 5:00 pm
Thursday .....7:30 am - 2:30 pm

Guest Registration ($10) includes designated name badge and entrance to the Sunday evening welcome reception. The badge does not gain entrance to oral sessions or the Poster/ Exhibit Hall.

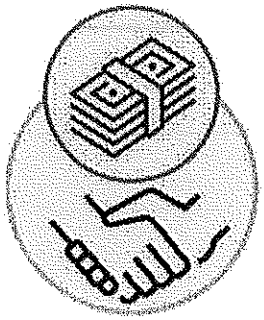
Gender Neutral Restrooms are designated in Building A and B, level three.

Mamava/Lactation Pods and Mother's Lounge
The center is equipped with two Mamava (lactation) pods, one in Building A (outside room A411) and one in Building B (across from B405). These pods are free for attendees to use. Meeting room B201 is also available for mothers to use.

Don't Miss these Resources in the Poster/Exhibit Hall

Bioinformatics Hub

- Learn from experts – designated times to come, ask questions, and get advice.
- Designated programs and debates to illuminate specific topics and tools.
- Look for schedule details on the hub's wiki (linked to www.asms.org) and entry sign at the conference.



Meet with representatives from various funding agencies. Appointment sign up sheets will be posted on 'office' entry sign. Attendees are encourage to take advantage of this valuable resource while at the conference.

Conference Regulations

Please review these policies which are intended to assure the comfort and privacy of all conference participants.

Name badge is required for all conference sessions, including the Poster/Exhibit Hall and Career Center, and off site events such as the hospitality suites and closing event (ticket required).

No smoking is permitted in the convention center.

All devices must be silenced and screens darkened in oral sessions.

No photography or recording is allowed in oral sessions or in the Poster/Exhibit Hall.

Parents. Planned conference sessions and hospitality suites may not be appropriate for children. Please respect the interests of your colleagues by allowing them to attend activities without disruption and without concern for the safety of children. Strollers, child backpack carriers or similar devices are permitted in the poster hall, and parents/caregivers are asked to keep in mind safety and well-being of children and conference attendees, taking care to avoid crowded spaces. Strollers are prohibited in the hospitality suites.

Material presented or displayed at the ASMS Conference, including but not limited to orals, posters, workshops, exhibit booths and hospitality suites, is the intellectual property of the presenter and may not be recorded, photographed, quoted, disseminated or transmitted by summary in any form without express written authority of the author.

The placement of advertising in the meeting area is prohibited. There are poster boards and tables in the Poster/Exhibit Hall for approved announcements.

Hardware, accessories or any items for sale may be displayed only in corporate exhibit booths and hospitality suites.

Designated publisher tables in the conference registration area are for the display of books and journals and must be reserved in advance.

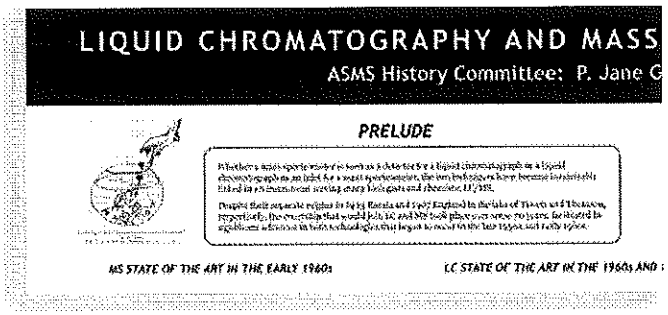
There are tables in the registration area for authors who wish to display their books. Authors may use a table to promote their books, sign copies, and speak with members. Table space must be reserved at conference registration.

No organized activities (even off-site) other than those approved by ASMS are allowed during the conference week (5:00 pm on Sunday through 6:00 pm on Thursday).

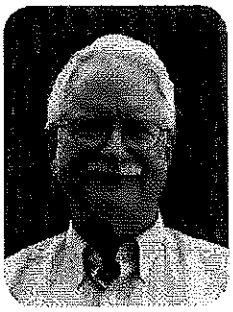
Corporate hospitality suites may be used during the daytime hours of 8:00 am - 8:00 pm for one-on-one and small group meetings (no more than 25 persons per organization) by appointment only (no walk-ins). No music, programs, seminars, or refreshments may be included in these private, business meetings.

Corporate or institutional logos on slides or posters may appear only one time in the presentation.

2019 Conference History Poster Display



Similar to previous years, the History Committee will again display a selection of posters that describe the historical development of our field and our Society with focus on key figures, pioneering instrument designs, and innovative applications of technology. We'll also continue the Vendor History theme initiated in 2018. This year's display will include vendor-created posters from last year plus two new ones: a second contribution from Waters highlighting the development of their quadrupole mass analyzers through the line of companies VG/Fisons/Micromass/Waters and one from Agilent describing quadrupole instrument development at Hewlett-Packard/Agilent. Finally, we'll celebrate ASMS's 60th birthday by re-displaying the anniversary decade posters for the years 1953-1992 and extending the series with two new additions: the 1993-2002 decade, "Biology Meets Mass Spectrometry," and the succeeding 2003-2012 decade, "The Era of 'Omics." Plan to spend some time with us at the History Poster Display in the main lobby/registration area!





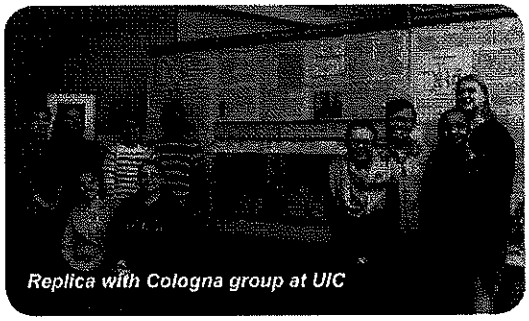
New Members of the History Committee

The History Committee welcomed two new members in 2018: Phil Price, a long-time ASTM E-14 and ASMS member whose work for the Society actively shaped the history of Standards and Nomenclature, and Glen Jackson, ASMS member since 2001 and a Fellow of the American Academy of Forensic Sciences who has written extensively on the history of Forensics Mass Spectrometry.

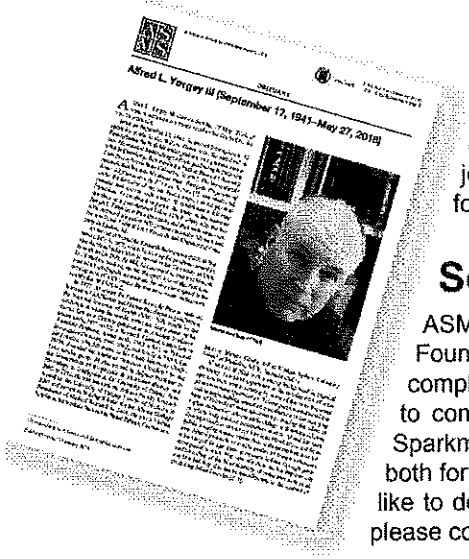
New History Committee members Phil Price (left) and Glen Jackson (right)

Historic Instrument Replicas

The Replica Display has a new home! After an 18-month stay at the University of Illinois at Chicago, jointly hosted by Professors Stephanie Cologna and Laura Sanchez, the Replica Display has moved to the University of Texas at Austin under the auspices of Professor Livia Eberlin. Read about the genesis of the Replica project, follow the display's itinerary, and learn how to add your institution to the list of future venues on its newly-created webpage (https://www.asms.org/about/history/historical-instruments-replica).



Replica with Cologna group at UIC



In Memoriam

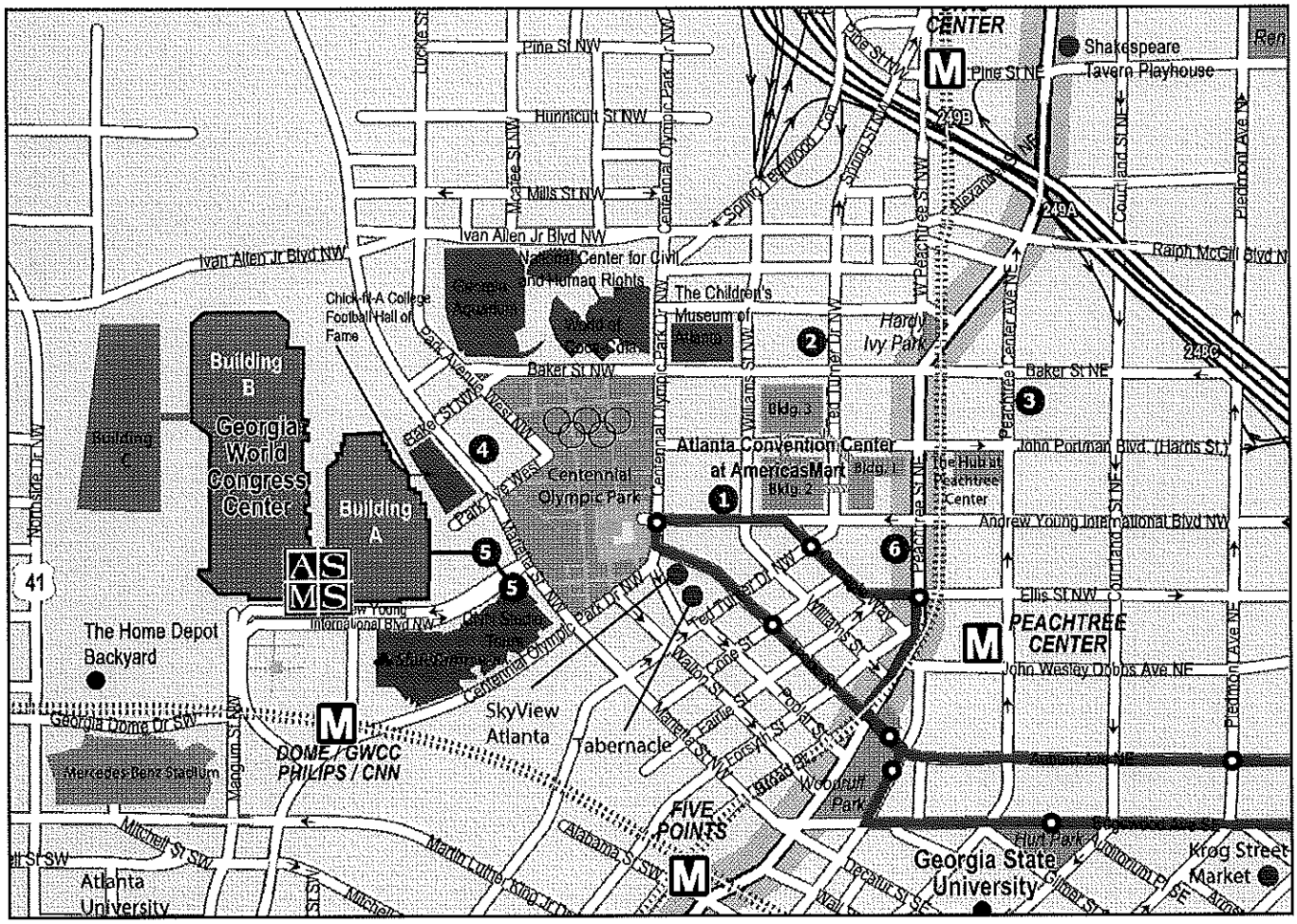
The ASMS website now contains links to JASMS articles that celebrate the lives of deceased ASMS members. Check out https://www.asms.org/publications/journal-of-the-american-society-for-mass-spectrometry-group/obituaries-from-jasms for remembrances of scientists whose work was seminal to the development of our field.

Science History Institute

ASMS continues to partner with the Science History Institute (formerly Chemical Heritage Foundation) to preserve the Society's history. As Oral Histories of ASMS members are completed and published, links to the full interviews are added to the History web page. Soon to come at https://www.asms.org/about/history/oral-history-project: Ron Macfarlane, David Sparkman and Jack Watson! The Institute also provides archival storage for ASMS ephemera, both for the Society and for its members. If you have documents of historical importance you'd like to donate – like meeting programs, instrument manuals, photographs or other artifacts – please contact ASMS Archivist/Historian Jane Gale (jane.pjgale@gmail.com).

CONFERENCE HOTELS

1	AC Hotel by Marriott Downtown	Tel. (404) 524-5555
2	Aloft Atlanta Downtown	Tel. (678) 515-0300
3	Atlanta Marriott Marquis	Tel. (404) 521-0000
4	Embassy Suites Atlanta	Tel. (404) 223-2300
5	Omni Atlanta Hotel at CNN Center	Tel. (404) 659-0000
6	Westin Peachtree Plaza	Tel. (404) 659-1400



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CONGRATULATIONS
to these members who were elected to the ASMS Board

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ASMS INTEREST GROUPS AND COMMITTEES

Interest Group Coordinators

Analytical Laboratory Managers	Samuel Macintosh David Quilici
Bioinformatics for MS	Isabel Bludau William Noble
Biotherapeutics	Andrew W. Dawdy Hao Zhang
Career Development	Lucinda Hittle Charles Veltri
Clinical Chemistry	Don Chace Candice Ulmer
Data Independent Acquisition	Hannes Röst Birgit Schilling
Drug Metabolism & Pharmacokinetics	Jonathan Josephs Brian Rago
Energy, Petroleum & Biofuels	Marianny Y. Combariza Amy McKenna
Environmental Applications	Imma Ferrer Andrew Ottens
Exposomics	Silvia Balbo Jarod Grossman
Flavor, Fragrance and Foodstuff	Melanie Downs James Redwine
Forensics & Homeland Security	Brittany Casey Chris Mulligan
FTMS	Melinda McFarland Matthew B. Renfrow
Fundamentals	Christian Bleiholder Alexandre Shvartsburg
H/D Exchange, Covalent Labeling & Cross Linking	Jim Bruce Kasper D. Rand
Imaging MS	Peggi Angel Martina Marchetti-Deschmann
Ion Mobility MS	Brian Clowers Valerie Gabelica
Ion Trap MS	Glen Jackson Desmond Kaplan
LC/MS Related Topics	Eric Soderblom Will Thompson
Lipids & Lipodomics	John A. Bowden Kim Ekroos
Metabolomics	Gary Patti Jon Sobus
Metal Ion Coordination Chemistry	Franklin Leach Nicolas Polfer
Oligonucleaotides & Nucleic Acids	Samuel Wainhaus Laixin Wang
Pharmaceuticals	Andrew W. Dawdy Richard Rogers
Photoionization MS	Sven Ehlert Matthias Lorenz Eleanor Riches
Polymeric Materials	Jessica Hoskins Christina Mastromatteo
Regulated Bioanalysis	Fabio Garofolo Jian Wang
Top-Down Proteomics	Frederik Lermyte Nicholas Young
Undergraduate Research in MS	Jay G. Forsythe Christine Hughey
Young Mass Spectrometrists	Veronica Anania Sharon Pitteri

Committees

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Digital Communications	Alexey Nesvizhskii, Chair Stephanie Cologna Desmond Kaplan Brendan MacLean Stacy Sherrod
Diversity	Livia Eberlin Fernandez Lima Francisco Lisa Jones Scott McLuckey Jessica Prenni Vicki Wysocki (ASMS Board Rep.)
Education	Erin Baker, Chair Peggi Angel Matt Crowe Sarah Robinson Laura Sanchez
History	P. Jane Gale, Chair Miriam ElNaggar Glen Jackson Phil Price Ken Tomer Michael Grayson, *ex-officio*
Nominating	Scott McLuckey, Chair Lucinda Hittle Hee-Yong Kim Sharon Pitteri
Publications	Amanda B. Hummon, Chair Theodore Alexandrov Peter Nemes Olga Ovchinnikova Candice Ulmer Joseph Loo, *ex officio*
Sanibel Conference	Melinda McFarland, Chair Leslie Hicks Shi Stone Kevin Bateman (ASMS Board Rep.)

JOHN B. FENN AWARD FOR A DISTINGUISHED CONTRIBUTION IN MASS SPECTROMETRY

2019 Recipient: John R. Yates III

Award Lecture: 4:45 PM, Monday, Murphy Ballroom, Building B, Level 5



The ASMS Award for Distinguished Contribution in Mass Spectrometry honors the memory of John B. Fenn who shared the 2002 Nobel Prize for the development of electrospray ionization. John joined ASMS in 1986 and remained an active member until his passing in 2010. The award is conferred at the ASMS Annual Conference with the presentation of a $10,000 cash award, a recognition plaque, and the award lecture.

Dr. John R. Yates III is the recipient of the 2019 ASMS John B. Fenn Award for a Distinguished Contribution in Mass Spectrometry, for development of automated, large-scale interpretation of peptide tandem mass spectral data. Dr. Yates' SEQUEST algorithm laid a critical foundation for the field of proteomics and has enhanced the accuracy and effectiveness of mass spectrometry to understand important biological and clinical questions.

Subsequent software developments continue to empower molecular and cellular biology research, including peptide and protein quantitation, identification of posttranslational modifications, and the use of DNA sequences to enable proteogenomic methods. Dr. Yates also enabled large-scale studies to identify the components of protein complexes in single celled organisms and mammalian cells. Proteomics is now practiced by thousands of researchers all over the world to study proteins in almost every organelle in prokaryotic and eukaryotic cells. The comprehensive analysis of cells and tissues is now routinely used to understand differences between normal and disease states.

Dr. Yates is Professor, Department of Molecular Medicine, The Scripps Research Institute.

AL YERGEY MS SCIENTIST AWARD

2019 Recipient: Jeffery Shabanowitz

Award presentation: 4:45 PM, Monday, Murphy Ballroom, Building B, Level 5



The Al Yergey Mass Spectrometry Scientist Award is sponsored by ASMS to recognize dedication and significant contributions to mass spectrometry-based science by "unsung heroes." This award is named in memory of Al Yergey a well-respected scientist who was known as a dedicated mentor.

Dr. Jeffrey Shabanowitz is the inaugural recipient of the Al Yergey MS Scientist Award. For more than forty years Dr. Shabanowitz has worked with Professor Donald Hunt at the University of Virginia, where he co-authored more than 330 peer-reviewed scientific papers and is co-inventor on ten issued patents. He played a major role in development of peptide sequence analysis by tandem mass spectrometry. The methods and instrumentation he helped to develop underpin the field of proteomics, and have led to major breakthroughs, especially in immunology and epigenetics research. He has also been a valued mentor to dozens of graduate students, postdocs, and visiting scientists. Dr. Shabanowitz is Principal Scientist in the Hunt Laboratory at the University of Virginia

BIEMANN MEDAL

2019 Recipient: Sarah Trimpin

Award Lecture: 4:45 PM, Tuesday, Murphy Ballroom, Building B, Level 5



The Biemann Medal is awarded to an individual early in his or her career to recognize significant achievement in basic or applied mass spectrometry. The Medal is conferred at the ASMS Annual Conference with the presentation of a $5,000 cash award, a recognition plaque, and the award lecture.

Dr. Sarah Trimpin is the recipient of the 2019 Biemann Medal for discovery and development of novel ionization processes. Dr. Trimpin's unusual observation of highly charged protein ions in an atmospheric pressure MALDI experiment led to her discovery that ionization occurs simply by passing compounds through the inlet of a mass spectrometer. She demonstrated that this simple approach achieves sensitivity comparable with, and frequently better than, electrospray or MALDI.

Through fundamental studies, Dr. Trimpin discovered solid matrices that produce highly charged ions upon laser ablation using MALDI ion sources. Even more astonishing is her discovery of matrix compounds that spontaneously produce multiply charged ions when exposed to vacuum (termed matrix-assisted ionization, MAI). No heat, nebulizing gases, laser, or voltage is required and exceptionally low chemical background is achieved for a variety of compounds, including proteins at least as large as bovine serum albumin (66 kDa). She has now discovered more than forty matrices that spontaneously produce analyte ions. Her work has been recognized by numerous awards and has led to commercialization.

Dr. Trimpin is Professor of Chemistry at Wayne State University.



2019 RESEARCH AWARDS

Award Presentations: 4:45 pm, Tuesday, Murphy Ballroom, Building B, Level 5

Research awards promote the research of academic scientists within the first four years of joining the tenure track or research faculty of a North American University at the time the award is conferred. The awards, in the amount of $35,000 each, are fully supported by Bruker, Thermo Fisher Scientific, and Waters Corporation.

Sponsored by
Bruker



James F. Davies
University of California, Riverside

Sponsored by
Thermo Fisher Scientific



Nicolas L. Young
Baylor College of Medicine

Sponsored by
Waters Corporation



Eleanor Browne
University of Colorado, Boulder

2019 PRIMARILY UNDERGRADUATE INSTITUTION RESEARCH AWARD

Award Presentations: 4:45 pm, Tuesday, Murphy Ballroom, Building B, Level 5

Sponsored by Agilent Technologies

This award promotes academic research in mass spectrometry by faculty members and their students at primarily undergraduate institutions (PUIs). The award of $20,000 is made to the recipient's institution on behalf of the recipient's research.

Callie Cole
Fort Lewis College



RON HITES AWARD FOR OUTSTANDING RESEARCH PUBLICATION IN *JASMS*

Award Presentations: ASMS Meeting, 4:45 pm, Wednesday, B302-305, Level 3



The Ron Hites Award recognizes an outstanding publication of original research based on innovative aspects, technical and presentation quality, and likely stimulation of future research or applications. The award is named to honor Professor Ron Hites of Indiana University, who led the creation of *JASMS* in 1988 while president of ASMS. The award includes $2,000 and certificates.

The 2019 Ron Hites Award recognizes Dr. Julia Laskin, Purdue University and her co-authors for their paper **Towards High-Resolution Tissue Imaging Using Nanospray Desorption Electrospray Ionization Mass Spectrometry Coupled to Shear Force Microscopy**; Son N. Nguyen, Ryan L. Sontag, James P. Carson, Richard A. Corley, Charles Ansong, and Julia Laskin; *J. Am. Soc. Mass Spectrom.* (2018) 29:316Y322.

2019 POSTDOCTORAL CAREER DEVELOPMENT AWARDS

Award Presentations: ASMS Meeting, 4:45 pm, Wednesday, B302-305, Level 3

Up to five awards in the amount of $5,000 each are intended to promote the professional career development of postdoctoral fellows in the field of mass spectrometry. Activities funded by these awards include conference and workshop attendance, travel to other mass spectrometry laboratories, purchase of books and/or software. The awards are open to ASMS members who are postdoctoral fellows within three years of completing a Ph.D. or equivalent degree. Applicants must be currently appointed as a postdoctoral fellow in North America (e.g., in academia, industry, a government or national laboratory or at a research institute). Details and an application are posted to asms.org.



Christopher Ashwood
Medical College of Wisconsin



Josue Baeza
University of Pennsylvania



Gongyu Li
University of Wisconsin-Madison



Jared Kafader
Northwestern University



Nicholas Riley
Stanford University

2019 STUDENT TRAVEL AWARDS

Award Presentations: ASMS Meeting, 4:45 pm, Wednesday, B302-305, Level 3

ASMS supports up to twenty awards of $1,000 for graduate students and ten awards of $500 for undergraduates. Applications and details for these awards are posted to asms.org.

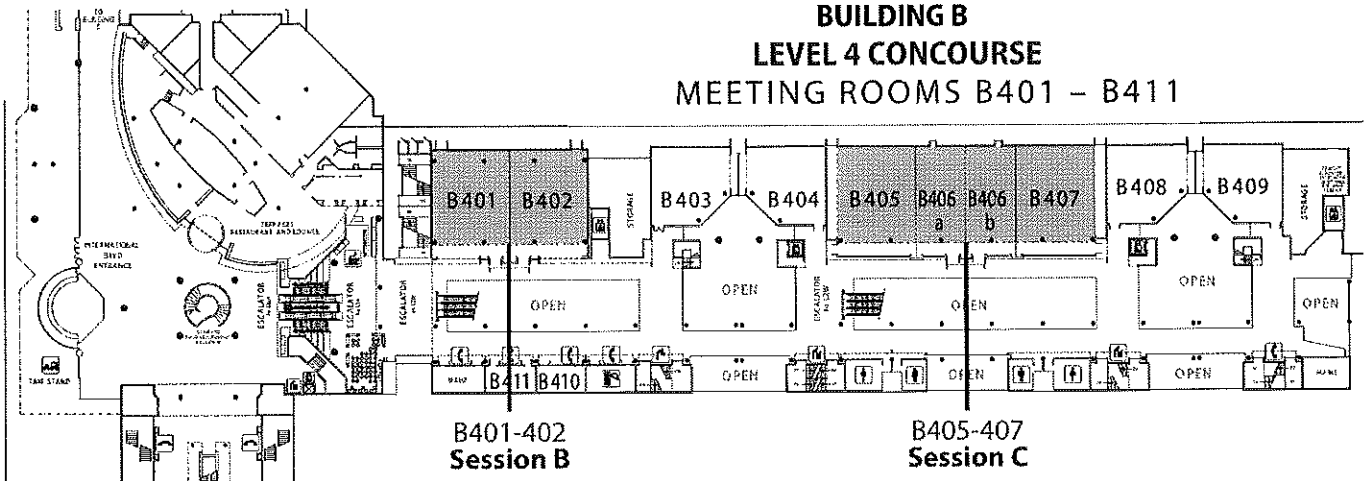
Graduate Student Awards

Molly Blevins, *University of Texas at Austin*
Wanying Cao, *University of Nebraska-Lincoln*
Ming Cheng, *Washington University in St.Louis*
Sean Cleary, *University of Oregon*
Mariel Coradin, *University of Pennsylvania*
Kellen DeLaney, *University of Wisconsin-Madison*
Kristen Fowble, *University at Albany-SUNY*
Naren Gajenthra Kumar, *Virginia Commonwealth University*
Praveen Kumar, *University of Minnesota*
Ting-Hao Kuo, *National Taiwan University*
Chenxi Liu, *University of Arizona*
Elijah McCool, *Michigan State University*
Sibylle Pfammatter, *IRIC-Université de Montréal*
Jaqueline A. Picache, *Vanderbilt University*
Erika Portero, *University of Maryland, College Park*
Marta Sans Escofet, *University of Texas at Austin*
Leah Schaffer, *University of Wisconsin-Madison*
Savannah Snyder, *The University of Akron*
Yang Tang, *Boston University*
Trisha Tucholski, *University of Wisconsin - Madison*

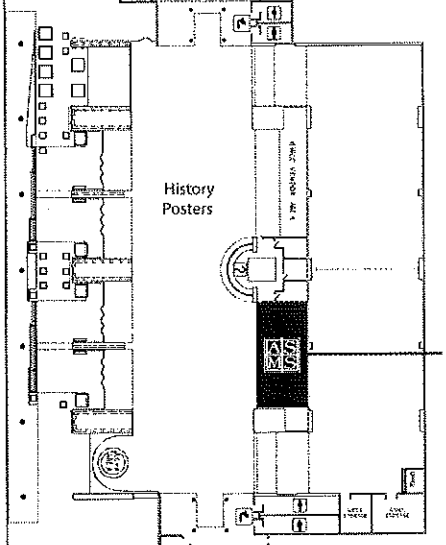
Undergraduate Student Awards

Shelby Beasley, *University of Oklahoma*
Alisha Birk, *Stanford University*
Cameron Davis, *National High Magnetic Field Laboratory*
Richard Dilworth, *University of Florida*
Anna Iacovino, *Duquesne University*
Kaylie Kirkwood, *North Carolina State University*
Abigail Lemmon, *University of Pennsylvania*
Javier Moreno, *Florida International University*
Amanda Wong, *Saint Mary's College of California*
Emily Ziperman, *Baylor University*

BUILDING B
LEVEL 4 CONCOURSE
MEETING ROOMS B401 – B411

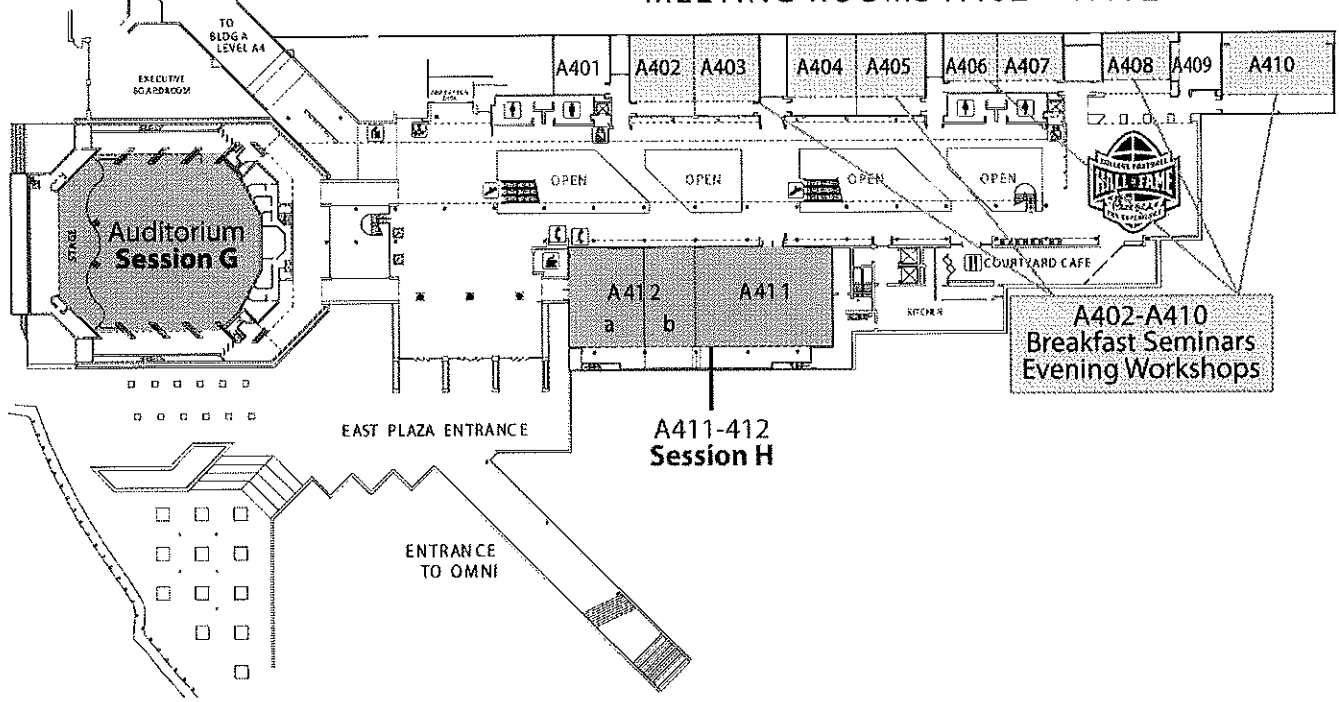


INTERNATIONAL BOULEVARD

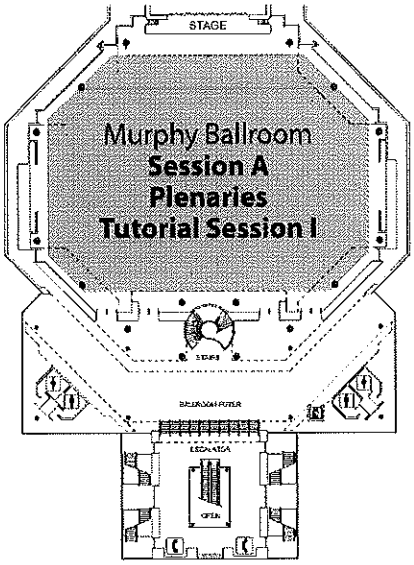


INTERNATIONAL BLVD. ENTRANCE

BUILDING A
LEVEL 4 CONCOURSE
MEETING ROOMS A402 – A412



INTERNATIONAL BOULEVARD



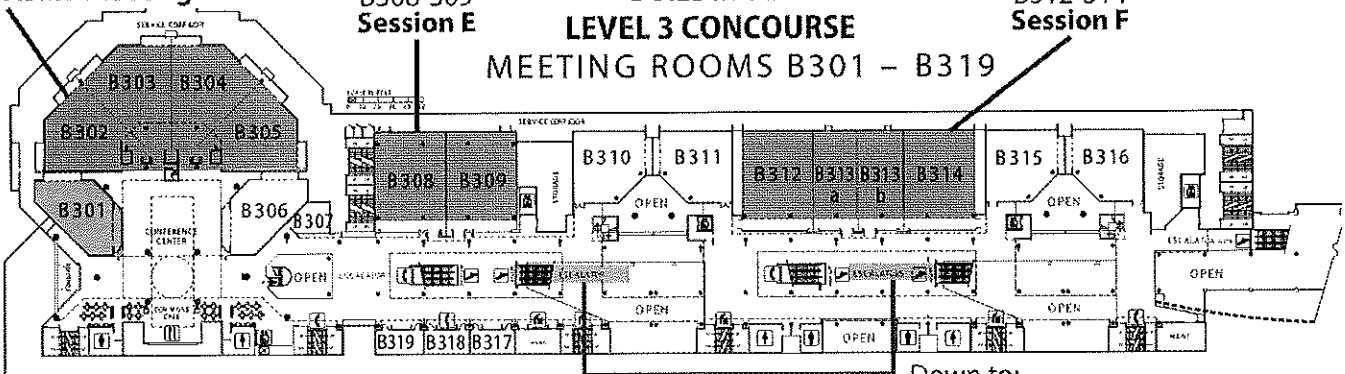
Thomas B. Murphy Ballroom
BUILDING B
Level 5 Concourse

B302-305
Session D
Tutorial Session II
ASMS Meeting

B308-309
Session E

BUILDING B
LEVEL 3 CONCOURSE
MEETING ROOMS B301 – B319

B312-314
Session F

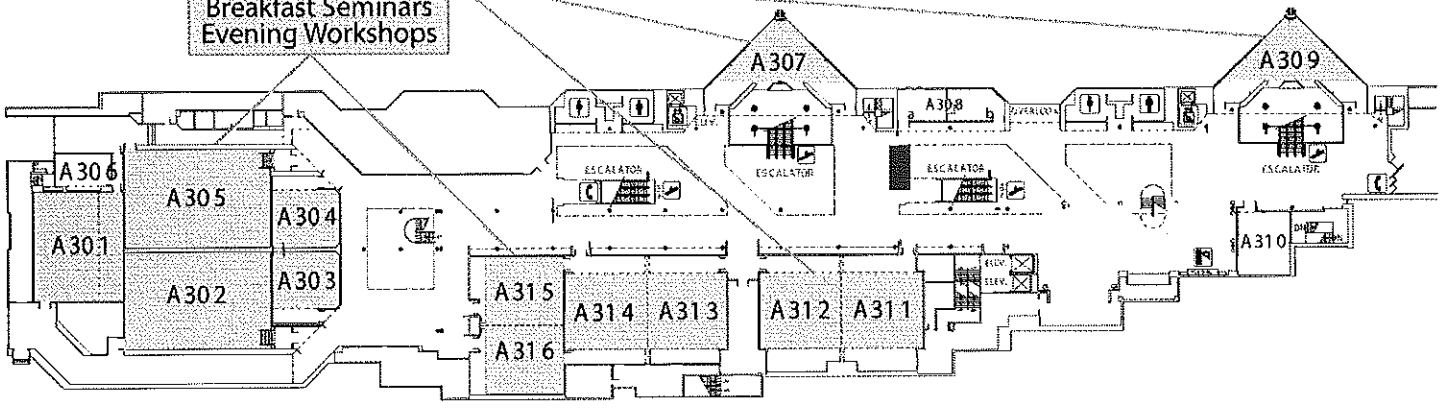


B301
Speaker Ready Room

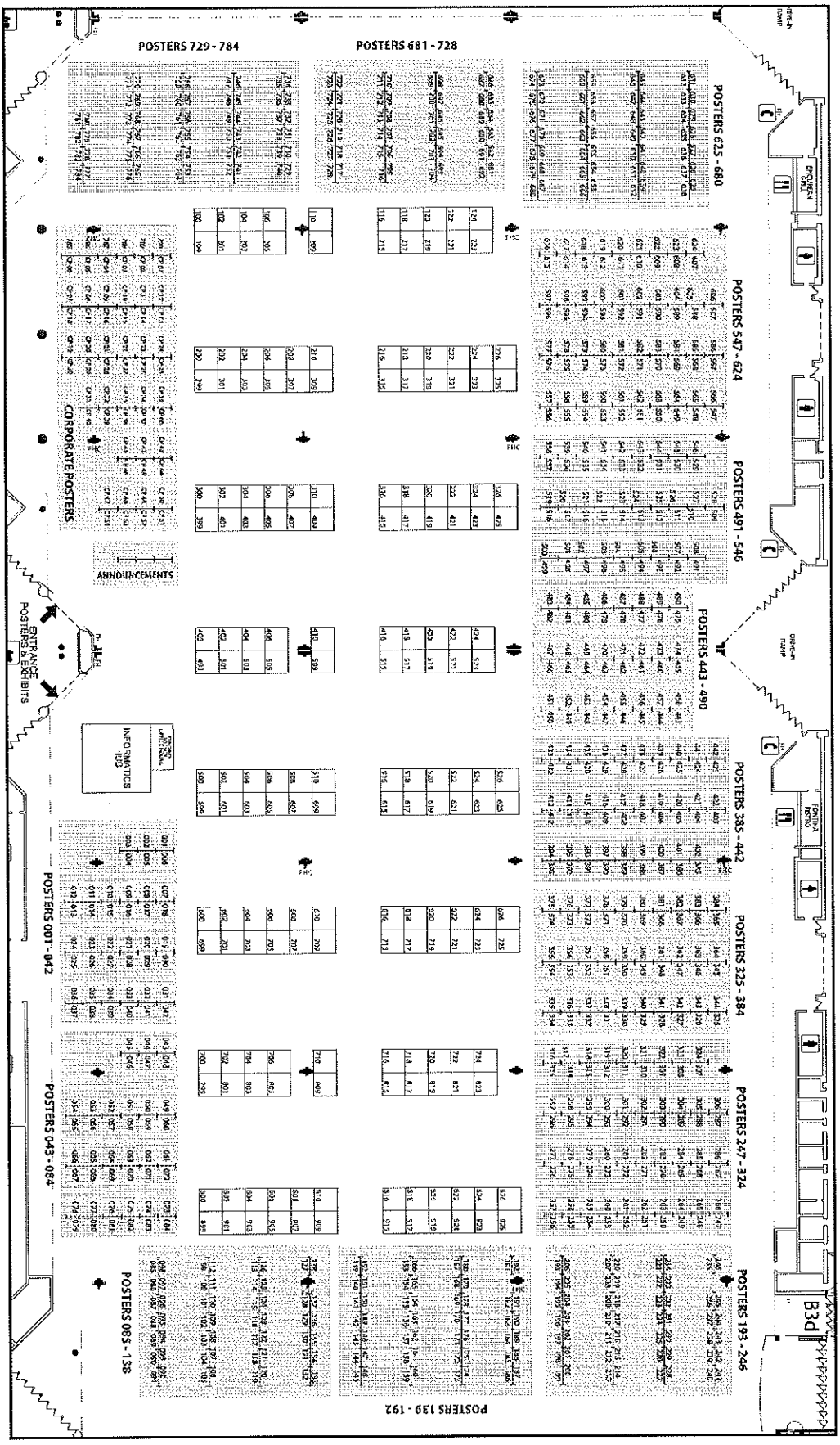
Down to:
B200 Meeting Rooms
Career Center
Exhibits / Posters

BUILDING A
LEVEL 3 CONCOURSE
MEETING ROOMS A301 – A316

A301-A316
Breakfast Seminars
Evening Workshops

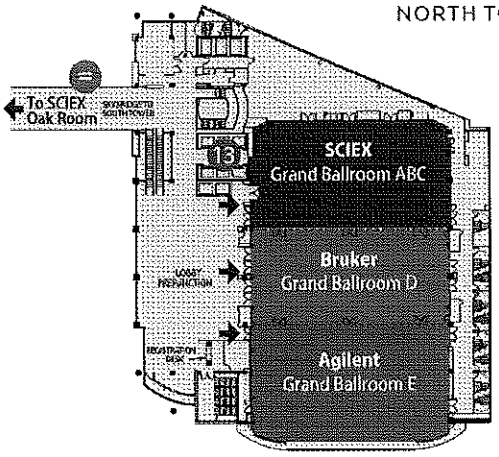


POSTER / EXHIBIT HALL

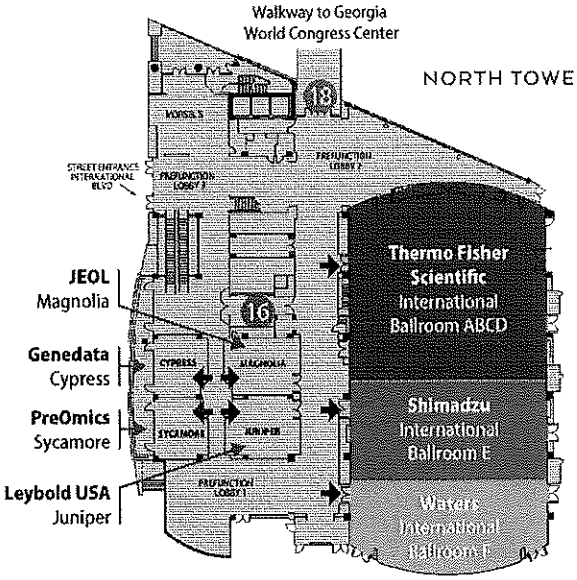


NORTH TOWER

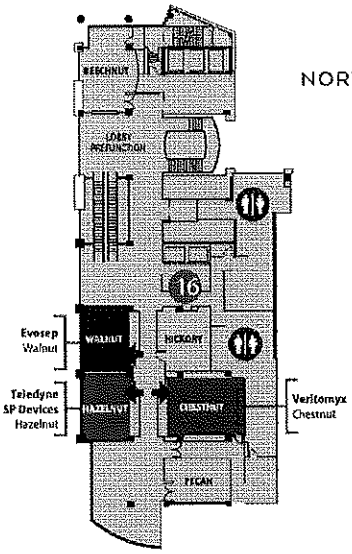
NORTH TOWER | M4



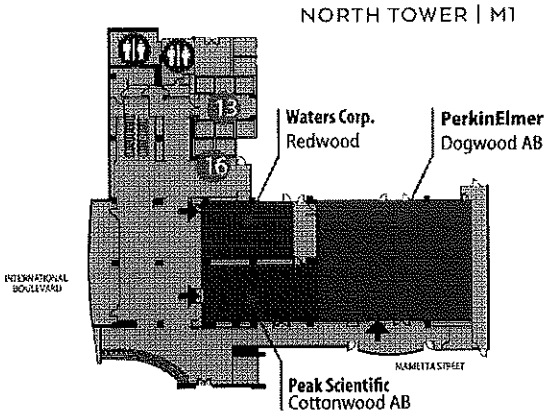
NORTH TOWER | M2



NORTH TOWER | M3



NORTH TOWER | M1



ELEVATORS
13 Guest Room Elevators (North Tower M1, M4, N6-28)
16 Meeting Room Elevators (North Tower M1-M4)

LANDMARKS
Skybridge
18 Walkway to Georgia World Congress Center and College Football Hall of Fame

RESTROOMS



HOSPITALITY SUITES 2019

In Atlanta hospitality suites will continue to embrace the back to basics atmosphere to allow attendees to learn more about the latest and greatest products and services of our Corporate Members while enjoying some fun, food and drink – *and conversation.*

Conference name badges are required for access to all conference activities including hospitality suites.

MEDIA EVENTS (PRESS CONFERENCES)

The following media events are scheduled **Monday, June 3** in the Omni CNN Center Hotel. All press are invited to attend these events.

8:00 - 9:00 am	Shimadzu Scientific Instruments	International Ballroom E
9:30 - 10:30 am	Bruker Daltonics	Grand Ballroom D
11:00 am - 12:00 pm	SCIEX	Grand Ballroom ABC
1:30 - 2:30 pm	Agilent	Grand Ballroom E
3:00 - 4:00 pm	Thermo Fisher Scientific	International Ballroom ABCD
4:30 - 5:30 pm	Waters Corporation	International Ballroom F

BREAKFAST SEMINARS

Breakfast seminars are hosted by Corporate Members at either the Convention Center or the Omni Hotel at CNN Center (inside hospitality suites). Pre-registration (RSVP) is recommended because room set-up and catering are arranged in advance. Please look for Breakfast Seminars page on www.asms.org and in the mobile app to find online registration links.

MONDAY BREAKFASTS

CONVENTION CENTER *All breakfast seminars begin at 7:00 am*	
Advanced Chemistry Development (ACD/Labs)	Room A313
Bruker Daltonics	Room A302
LECO Corporation	Room A314
MassTech Inc.	Room A315
Matrix Science	Room A410
Pressure BioSciences Inc.	Room A312
SCIEX (3)	Rooms A404-405, A406-407, A408
Shimadzu Scientific Instruments	Room A305
Waters Corporation	Room A402-403
OMNI HOTEL AT CNN CENTER	
Agilent Technologies	Grand Ballroom E
Thermo Fisher Scientific	International Ballroom ABCD
Waters Corporation	International Ballroom F

TUESDAY BREAKFASTS

CONVENTION CENTER *All breakfast seminars begin at 7:00 am*	
Biognosys	Room A312
Biotage	Room A316
Bruker Daltonics	Room A302
Evosep	Room A311
Genedata	Room A315
LECO Corporation	Room A314
Matrix Science	Room A410
New Objective Inc.	Room A313
SCIEX (3)	Rooms A404-405, A406-407, A408
Shimadzu Scientific Instruments	Room A305
Waters Corporation	Room A402-403
OMNI HOTEL AT CNN CENTER	
Agilent Technologies	Grand Ballroom E
Thermo Fisher Scientific	International Ballroom ABCD
Waters Corporation	International Ballroom F

WEDNESDAY BREAKFASTS

CONVENTION CENTER *All breakfast seminars begin at 7:00 am*	
Avanti Polar Lipids	Room A410
Bruker Daltonics	Room A302
LECO Corporation	Room A314
MassTech Inc.	Room A315
New Objective Inc.	Room A313
SCIEX (3)	Rooms A404-405, A406-407, A408
Shimadzu Scientific Instruments	Room A305
OMNI HOTEL AT CNN CENTER	
Agilent Technologies	Grand Ballroom E
Thermo Fisher Scientific	International Ballroom ABCD
Waters Corporation	International Ballroom F

THURSDAY BREAKFASTS

CONVENTION CENTER *All breakfast seminars begin at 7:00 am*	
MassTech Inc.	Room A315
SCIEX (3)	Rooms A404-405, A406-407, A408
Shimadzu Scientific Instruments	Room A305
Thermo Fisher Scientific	Room A302





ASMS CORPORATE MEMBERS

Corporate Member	Exhibit Booth	Corporate Poster or Publisher Tabletop	Hospitality Suite at at Omni Hotel at CNN Center	Breakfast Seminar
908 Devices	802	Corporate Poster		
AcroMass Technologies, Inc.	724			
ACS Publications	919			
Adaptas Solutions	216	Corporate Poster		
Advanced Chemistry Development (ACD/Labs)	316	Corporate Poster		Conv Ctr Room A313: Mon 6/3
Advion	718			
Agilent Technologies	400	Corporate Poster	Grand Ballroom E	Omni Grand Ballroom E: Mon-Wed (6/3-6/5);
AIM Research Company	224			
Alliance Pharma	202			
Analytical Sales and Services, Inc.	302	Corporate Poster		
Analytical Scientific Instruments US Inc.	318			
Antec Scientific	505	Corporate Poster		
APEX - Alberta Precision Exchange	222			
Apricot Designs	522	Corporate Poster		
ASTA	617	Corporate Poster		
Avanti Polar Lipids, Inc.	199			Conv Ctr Room A410: Wed 6/5
Baran Bioscience, LLC		Corporate Poster		
BaySpec, Inc.	220			
Beckman Coulter	818			
BGI	703			
Bioanalysis Zone	219			
BioChromato	208	Corporate Poster		
Biocrates Life Sciences AG	706			
Biognosys	517			Conv Ctr Room A312: Tue 6/4
Bioinformatics Solutions Inc.	409	Corporate Poster		
Biotage	526			Conv Ctr Room A316: Tues 6/4
Biotech Support Group	719			
Bruker Daltonics	515	Corporate Poster	Grand Ballroom D	Conv Ctr Room A302: Mon-Wed (6/3-6/5)
Cambridge Isotope Laboratories, Inc.	502			
Cayman Chemical Company	710	Corporate Poster		
Cerno Bioscience	909			
ChemoPower Technology	819			
Coann Technologies	423			
Compare Networks		Publisher's Tabletop		
CovalX	299			
CSS Analytical Co. Inc				
CTC Analytics AG	519			
Ebara Technologies	419	Corporate Poster		
Edwards Vacuum	705			
El-Mul Technologies	301			



ASMS CORPORATE MEMBERS

Corporate Member	Exhibit Booth	Corporate Poster or Publisher Tabletop	Hospitality Suite at at Omni Hotel at CNN Center	Breakfast Seminar
e-MSion, Inc.	424			
Entech Instruments	826			
ESI Source Solutions	116			
Evosep	518		Walnut	Conv Ctr Room A311: Tue 6/4
Extrel CMS	325			
Fasmatech	717			
F-DGSi	803			
Fossil Ion Technology	704	Corporate Poster		
Genedata	510	Corporate Poster	Cypress	Conv Ctr Room A315: Tue 6/4
Genetic Engineering & Biotechnology News		Publisher's Tabletop		
GenNext Technologies, Inc.	816			
Genovis Inc	323	Corporate Poster		
GenTech Scientific, Inc.	317			
GERSTEL, Inc.	716			
GL Sciences	215			
Grenova	509			
Hamamatsu Corporation	110	Corporate Poster		
Hamilton Company	307	Corporate Poster		
Harris Corporation	604	Corporate Poster		
HILICON AB		Corporate Poster		
HTX Technologies, LLC	404			
HVM Technology, Inc.	622			
IDEX Health & Science	402	Corporate Poster		
IMCS	305			
Imtakt USA	406			
Institute for Systems Biology	118			
Intavis, Inc	722			
INTEGRA Biosciences	610			
International Ceramic Engineering	217			
International Equipment Trading Ltd	602			
International Labmate Ltd.		Publisher's Tabletop		
Ion Opticks Pty Ltd	524			
IonBench	226			
IONICON	799	Corporate Poster		
Ionoptika Ltd.	707			
Ionsense Inc.	506	Corporate Poster		
IONTOF GmbH	425			
IP2	801			
IROA Technologies LLC	223			
IsoSciences	421			
JASMS	915			
JEOL USA, Inc.	200		Magnolia	



ASMS CORPORATE MEMBERS

Corporate Member	Exhibit Booth	Corporate Poster or Publisher Tabletop	Hospitality Suite at at Omni Hotel at CNN Center	Breakfast Seminar
JG Finneran Associates, Inc.	310			
Kashiyama USA	804			
Kura Biotech Inc.	620	Corporate Poster		
Lab Tech Support	322			
Larodan AB	221			
LCGC/Spectroscopy	702			
LECO Corporation	401	Corporate Poster		Conv Ctr Room A314: Mon-Wed (6/3-6/5)
Leybold USA	403		Juniper	
Linden CMS GmbH	721			
LNI Swissgas	806	Corporate Poster		
MAC-MOD Analytical	720			
MasCom Technologies	615			
MassTech Inc.	624			Conv Ctr Room A315: Mon 6/3, Wed-Thurs (6/5-6/6)
MathSpec, Inc.		Corporate Poster		
Matrix Science	523			Conv Ctr Room A410: Mon-Tue (6/3-6/4)
Matsusada Precision Inc	815			
McKinley Scientific	605			
MDC Vacuum Products LLC	203			
Merck - DUE				
MetaSci Inc.	817			
Microsaic Systems plc	618	Corporate Poster		
Moeller Medical GmbH	810			
Mott Corporation	405	Corporate Poster		
MPF Products Inc	410			
MRM Proteomics	124			
MS Bioworks	319			
MS Ekspert	306			
MS Noise	626			
MSTM, LLC	601			
Nacalai USA	422	Corporate Poster		
National Institute of Standards and Technology (NIST)	616			
Nest Group, Inc., The		Corporate Poster		
New England Biolabs	901			
New England Peptide Inc.	417			
New Objective Inc.	324			Conv Ctr Room A313: Tue-Wed (6/4-6/5)
Newomics Inc.	606			
Novatia LLC		Corporate Poster		
Omics Informatics LLC	321			
Omni International	415			
OMNI Lab Solutions	418	Corporate Poster		



ASMS CORPORATE MEMBERS

Corporate Member	Exhibit Booth	Corporate Poster or Publisher Tabletop	Hospitality Suite at at Omni Hotel at CNN Center	Breakfast Seminar
Opentrons	905			
Optimize Technologies	700	Corporate Poster		
Parker Hannifin	805			
Peak Scientific	699	Corporate Poster	Cottonwood AB	
PerkinElmer, Inc.	899		Dogwood AB	
Pfeiffer Vacuum	599	Corporate Poster		
Pharmafluidics	303	Corporate Poster		
Phenomenex	508			
Phoenix S&T, Inc.	503			
PHOTONIS	609	Corporate Poster		
Phytronix Technologies	300			
Polymer Factory	520	Corporate Poster		
PreOmics GmbH	407		Sycamore	
Pressure BioSciences Inc.	823			Conv Ctr Room A312: Mon 6/3
Prolab Instruments GmbH	709	Corporate Poster		
Promega Corporation	315			
PROMISE Advanced Proteomics	201	Corporate Poster		
Protein Metrics Inc.	416			
Proteome Software Inc.	725			
PURSPEC Technologies Inc.	218			
Rapid Novor Inc.	723	Corporate Poster		
Ray Biotech	625			
Regeneron Pharmaceuticals	102			
Regis Technologies	808			
Restek Corporation	210			
ReSyn Biosciences	623	Corporate Poster		
SamIn Science Co. Ltd.	309			
Sciencix	106			
SCIEX	500		Grand Ballroom ABC & Oak Room	Conv Ctr Room A404-405: Mon-Thurs (6/3-6/6); Conv Ctr Room A406-407: Mon-Thurs (6/3-6/6); Conv Ctr Room A408: Mon-Thurs (6/3-6/6)
Shimadzu Scientific Instruments, Inc.	499	Corporate Poster	International Ballroom E	Conv Ctr Room A305: Mon-Thurs (6/3-6/6)
Shodex, Showa Denko America	304			
Sierra Analytics, Inc.	206	Corporate Poster		
Silantes GmbH	608			
SoCal Bioinformatics, Inc.	715			
Sound Analytics	701			
Spark Holland	603			
SpectralWorks	504	Corporate Poster		
Spectroswiss	516			
Spellman High Voltage Electronics Corp.	420			

ASMS CORPORATE MEMBERS

Corporate Member	Exhibit Booth	Corporate Poster or Publisher Tabletop	Hospitality Suite at at Omni Hotel at CNN Center	Breakfast Seminar
SPEX SamplePrep LLC	308			
SunChrom GmbH	209			
Synpeptide Co., Ltd.	607			
Tecan	800			
Teledyne SP Devices		Corporate Poster	Hazelnut	
Teledyne Tekmar	320			
The Analytical Scientist		Publisher's Tabletop		
Thermo Fisher Scientific	600		International Ballroom ABCD	Omni International Ballroom ABCD: Mon-Wed (6/3-6/5); Conv Ctr Room A302: Thurs 6/6
Tosoh Bioscience LLC	326			
Trajan Scientific and Medical	100	Corporate Poster		
Veritomyx	809		Chestnut	
VICI Valco Instruments	204	Corporate Poster		
VRS Recruitment	501			
Waters Corporation	399	Corporate Poster	International Ballroom F & Redwood	Omni International Ballroom F: Mon-Wed (6/3-6/5); Conv Ctr Room A402-403: Mon-Tue (6/3-6/4)
XP Power LLC	205			
Xtreme Power	521			
Zef Scientific, Inc.	621			
Zhejiang Haochuang Biotech Co. Ltd.	619			



PROGRAM ACKNOWLEDGEMENTS

VICE PRESIDENT FOR PROGRAMS



Susan Richardson
University of South Carolina
Vice President for Programs

STUDENT ASSISTANTS

Graduate students assist with many aspects of the conference, including registration, oral and poster sessions, and the employment center. The students each receive a stipend to help with their conference travel expenses.

PROGRAM COMMITTEE

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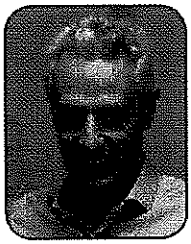
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Benedikt Warth
Ian Webb
Si Wu
Nicolas Young
Hao Zhang

SATURDAY

9:00 AM - 4:30 PM	**SHORT COURSES**
2:00 - 5:00 PM	**REGISTRATION,** Building B Main Lobby

SUNDAY

9:00 AM - 4:30 PM	**SHORT COURSES**
10:00 AM - 8:00 PM	**REGISTRATION,** Building B Main Lobby
4:00 - 4:45 PM	**ATTENTION: FIRST-TIME GRADUATE STUDENTS AND UNDERGRADUATE STUDENTS** **Plan your Strategy: What to See and Do at ASMS,** B302-305, Level Three
5:00 - 6:30 PM	**TUTORIAL SESSION I,** Murphy Ballroom, Bldg. B, Level Five **5:00 - 5:45 pm** **Lipidomics** **Stephen Blanksby,** *Queensland U. of Technology* **& Gavin Reid,** *University of Melbourne*   **5:45 - 6:30 pm** **Targeted Imaging** **Enrico Davoli** *Mario Negri Institute*  **TUTORIAL SESSION II,** B302-305, Level Three **5:00 - 5:45 pm** **Native Mass Spectrometry** **Michal Sharon** *Weizmann Institute*  **5:45 - 6:30 pm** **Data Independent Acquisition** **Birgit Schilling** *The Buck Institute* 
6:45 - 7:45 PM	**CONFERENCE OPENING,** Murphy Ballroom, Bldg. B, Level Five **Susan Richardson,** *University of South Carolina* ASMS Vice President for Programs  **7:00 - 7:45 pm** **Transitioning the World Energy for All Purposes to Stable Electricity Powered by 100% Wind, Water, and Sunlight** **Mark Z. Jacobson** *Stanford University*
7:45 - 9:00 PM	**WELCOME RECEPTION IN THE POSTER/EXHIBIT HALL** Undergraduate Student Poster Competition

MONDAY

7:00 AM	**CORPORATE BREAKFAST SEMINARS,** Convention Center and Omni CNN Center Hotel
7:30 AM - 5:00 PM	**REGISTRATION,** Building B Main Lobby
8:30 - 10:30 AM	**ORAL SESSIONS** MOA am: Cannabis Testing, *Murphy Ballroom, Bldg. B, Level Five* MOB am: Glycopeptides and Glycoproteins, *B401-402* MOC am: Membrane Protein MS, *B405-407* MOD am: Imaging: Instrumentation & Method Development, *B302-305* MOE am: Lipidomics: Targeted and Untargeted, *B308-309* MOF am: Fundamentals: Ion Mobility and MS (In Memory of Al Yergey), *B312-314* MOG am: Instrumentation: Portable and Transportable Mass Spectrometers, *Auditorium, Bldg. A* MOH am: Biomarkers: Qualitative Analysis, *A411-412*
10:30 AM - 2:30 PM	**POSTER SESSION AND EXHIBITS,** Monday Posters, Poster/Exhibit Hall ground level **Odd-number posters present:** 10:30 - 11:30 am PLUS 12:30 – 2:30 pm **Even-number posters present:** 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm 11:30 am - 1:00 pm: **Undergraduate students** look for reserved tables and free lunch vouchers to ***Meet the Experts***
2:30 - 4:30 PM	**ORAL SESSIONS** MOA pm: Informatics: Multiomics Integration and Applications, *Murphy Ballroom, Bldg. B* MOB pm: Homeland Security: Chemical/Biological Defense, *B401-402* MOC pm: Food Safety & Chemistry: Foodomics, Allergens, Bacteria, Foods, and Supplements, *B405-407* MOD pm: Therapeutic Proteins, Antibodies, and Antibody/Drug Conjugates, *B302-305* MOE pm: Lipidomics: New MS Technologies and Applications , *B308-309* MOF pm: Biomarkers: Quantitative Analysis, *B312-314* MOG pm: Instrumentation: New Developments in Ionization and Sampling, *Auditorium, Bldg. A* MOH pm: Art, Archaeology, and Paleontology, *A411-412*
4:45 - 5:30 PM	**AWARD LECTURE,** Murphy Ballroom, Bldg. B, Level Five  **Award for a Distinguished Contribution in Mass Spectrometry** **John R. Yates III** *The Scripps Research Institute*
5:45 - 7:00 PM	**WORKSHOPS** There are light refreshments in Building A foyers, 5:30 - 5:45 pm. 01. High Spatial Resolution 2D and 3D Mass Spectrometry Analysis: Current Trends, *A402-403* 02. Enhancing MS-Based Glycomics and Glycoproteomics Toolbox: Round-table Discussion, *A404-405* 03. MassIVE Translation of Public Mass Spectrometry Big Data into Reusable Community Resources, *A406-407* 04. Mass Spectrometry in the Developing World: Supporting Education and Research, *A408* 05. Ion Trap Mass Spectrometry: Latest Trends (Ion Trap MS Interest Group), *A410* 06. FAIMS/DIMS/DMS Technology and its Impact on Current Day MS Analyses, *A307* 07. Food Safety and Quality Applications: Tools for Putting MS Methods into Practice (Flavor Frangrance & Foodstuff Interest Group), *A309* 08. Automation for Proteomics Sample Preparation, *A311* 09. MS Software: Peak Picking - Paramount Practices and Perilous Pitfalls, *A312* 10. Solid Phase Microextraction Approaches Applied with Mass Spectrometry Techniques, *A313* 12. LC-MS Jeopardy - I'll Take Increasing Throughput for $200 (LCMS & Related Topics Interest Group), *A315* 13. Art and Cultural Heritage: Mass Spec Applications, *A316* 14. Photoionization (APPI/PI) - Bridging the Gap between Academic and Industrial Research (Photoionization MS Interest Group), *A303* 15. MS-Based Multi-Attribute Method (MAM): The Future of Biotherapeutic Development Analytics (Biotherapeutics Interest Group), *A302* 16. MS Career Options: How to Kick Start Your Career (Young Mass Spectrometrists Interest Group), *A301* 17. Membrane Proteins, Nanodiscs, and Beyond: MS Analysis in Academia and Industry, A305 18. Energy, Petroleum, and Biofuels MS: Targeted Analysis, Fingerprinting and Speciation in Complex Mixtures (Energy Petroleum & Biofuels Interest Group), *A304*
7:00 - 8:00 PM	**DINNER BREAK**
AFTER 8:00 PM	**CORPORATE HOSPITALITY SUITES,** Omni CNN Center Hotel

TUESDAY

7:00 AM	**CORPORATE BREAKFAST SEMINARS,** Convention Center and Omni CNN Center Hotel
7:30 AM - 5:00 PM	**REGISTRATION,** Building B Main Lobby
8:30 - 10:30 AM	**ORAL SESSIONS** TOA am: Informatics: Innovations, *Murphy Ballroom, Bldg. B, Level Five* TOB am: Fundamentals: Photoionization and Photodissociation, *B401-402* TOC am: Native MS in Structural Biology, *B405-407* TOD am: Imaging: Pharmaceuticals, Metabolites, and Lipids, *B302-305* TOE am: Environmental: Emerging Contaminants (In Honor of Ron Hites), *B308-309* TOF am: Protein-Ligand Interactions, *B312-314* TOG am: MS in the QC Lab, *Auditorium, Bldg. A* TOH am: Nucleic Acids and Oligonucleotides, *A411-412*
10:30 AM - 2:30 PM	**POSTER SESSION AND EXHIBITS,** Tuesday Posters, Poster/Exhibit Hall ground level **Odd-number posters present:** 10:30 - 11:30 am PLUS 12:30 – 2:30 pm **Even-number posters present:** 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm
2:30 - 4:30 PM	**ORAL SESSIONS** TOA pm: Informatics: Data-Independent Acquisition, *Murphy Ballroom, Bldg. B, Level Five* TOB pm: GC/MS, GCxGC/MS, GC-MS/MS, and GC/HRMS, *B401-402* TOC pm: Top Down Protein Analysis, *B405-407* TOD pm: Drug Target Identification by MS, *B302-305* TOE pm: Food Safety & Chemistry: Innovations, *B308-309* TOF pm: Cancer Research, *B312-314* TOG pm: Instrumentation: Innovative Separations Approaches Coupled to MS, *Auditorium, Bldg. A* TOH pm: Energy, Petroleum, and Biofuels: Instrumentation and Applications, *A411-412*
4:45 - 5:30 PM	**AWARD LECTURE,** Murphy Ballroom, Bldg. B, Level Five  **Biemann Medal** **Sarah Trimpin** *Wayne State University*
5:45 - 7:00 PM	**WORKSHOPS** There are light refreshments in Building A foyers, 5:30 - 5:45 pm. 01. Top Down Proteomics: Advancing Widespread Adoption and Expanding Applications (Top-Down Proteomics Interest Group), *A402-403* 02. Networking for Scientists: Celebrating Women Mass Spectrometrists (Year 2), *A404-405* 03. Say No to Drugs: Forensic Applications Outside of Traditional Illicit Drug Analysis (Forensics & Homeland Security Interest Group), *A406-407* 04. Proteoform Identification and Quantification Using Toppic Suite, *A408* 05. Protein Biomarkers Method Development & Validation by LCMS, HRMS and Hybrid LBA/LCMS: Recent Advancements (Regulated Bioanalysis Interest Group), *A410* 06. Improving Scientific Writing Skills, *A307* 07. Metal Ions and Non-Threshold Ion Activation in Biomolecules (Metal Ion Coordination Chemistry Interest Group), *A309* 08. Protein Imaging - Are We There? Are All Issues Solved? (Imaging MS Interest Group), *A311* 09. Metabolomics: Points of Agreement and Disagreement (Metabolomics Interest Group), *A312* 10. Environmental MS: Detection of Emerging Contaminants (Environmental Applications Interest Group), *A313* 11. Visualization, Comparison and Accessibility of Large Data Sets (Analytical Lab Managers Interest Group), *A314* 12. Advances in Polymer Mass Spectrometry - Architecture (Polymeric Materials Interest Group), *A315* 13. (Emotional) Intelligence Gathering (Career Development Interest Group), *A316* 14. MS in Extractable and Leachable Analysis, *A303* 15. HDX, Covalent Labeling & Cross-Linking: Status of Community-Initiatives and New Developments and Applications (HDX Covalent Labeling & Cross Linking Interest Group), *A302* 16. Lipidomics: Path to Clinical Utility (Lipids & Lipodomics Interest Group), *A301* 17. Data Independent Acquisition: Expanding the Scope of DIA Strategies for Quantitative Mass Spectrometry (Data Independent Acquisition Interest Group), *A305* 18. Trans-Proteomic Pipeline: Recent Advances and Future Directions, *A304*
7:00 - 8:00 PM	**DINNER BREAK**
AFTER 8:00 PM	**CORPORATE HOSPITALITY SUITES,** Omni CNN Center Hotel

WEDNESDAY

7:00 AM	**CORPORATE BREAKFAST SEMINARS,** Convention Center and Omni CNN Center Hotel
7:30 AM - 5:00 PM	**REGISTRATION,** Building B Main Lobby
8:30 - 10:30 AM	**ORAL SESSIONS** WOA am: Metabolomics: New Technologies and Applications, *Murphy Ballroom, Bldg. B, Level Five* WOB am: Carbohydrates, *B401-402* WOC am: Fundamentals for Everyone: Peptides and Proteins, *B405-407* WOD am: Microdosing and Microsampling: Analytical Challenges, *B302-305* WOE am: Environmental: Innovative Approaches and Instrumentation, *B308-309* WOF am: Ion Mobility: New Developments & Applications, *B312-314* WOG am: Fundamentals for Everyone: Structural elucidation, *Auditorium, Bldg. A* WOH am: Synthetic Polymers, *A411-412*
10:30 AM - 2:30 PM	**POSTER SESSION AND EXHIBITS,** Wednesday Posters, Poster/Exhibit Hall ground level **Odd-number posters present:** 10:30 - 11:30 am PLUS 12:30 – 2:30 pm **Even-number posters present:** 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm
2:30 - 4:30 PM	**ORAL SESSIONS** WOA pm: Metabolomics: Untargeted Profiling, *Murphy Ballroom, Bldg. B, Level Five* WOB pm: Hydrogen-Deuterium Exchange MS: Innovations, *B401-402* WOC pm: Forensics: Innovations and Applications, *B405-407* WOD pm: Endogenous Protein Biomarkers in Drug Discovery and Development: Quantitative Analysis, *B302-305* WOE pm: Clinical Analysis: MS in the Operating Room, *B308-309* WOF pm: Ion Mobility: Small Molecules, Pharmaceuticals, and DMPK, *B312-314* WOG pm: Instrumentation: Ambient Ionization & Applications, *Auditorium, Bldg. A* WOH pm: Fundamentals: DDA and DIA LC-MS, *A411-412*
4:45 - 5:30 PM	**ASMS MEETING,** B302-305, Level Three: Awards, board reports, wine, beer, soft drinks - and more!
5:45 - 7:00 PM	**WORKSHOPS** There are light refreshments in Building A foyers, 5:30 - 5:45 pm. 01. MS-Based Interactomics: Computational Resources and Tools for Studying the Physical Interactome (Bioinformatics MS Interest Group), *A402-403* 02. IMS: When Chromatography Just Won't Do (Ion Mobility MS Interest Group), *A404-405* 03. Clinical Applications: Standardization and Harmonization Efforts (Clinical Chemistry Interest Group), *A406-407* 04. Exposomics Workshop (Exposomics Interest Group), *A408* 05. MS-Based Process Analytical Technology (PAT): Testing & Control of CQAs (Pharmaceuticals Interest Group), *A410* 06. Endogenous Biomarkers: Measurement to Predict in vivo Drug-Drug Interactions (DMPK Interest Group), *A307* 07. The NIH and NSF Review and Funding Process, *A309* 08. Why You Should Submit Your Best Manuscripts to JASMS (and Introducing a New Publisher), *A311* 09. Metaproteomics for the Masses: Solutions, Opportunities and Challenges, *A312* 10. Bridging the Gap between Computational Biology and Biology: Matchmaking Session, *A313* 11. Ambient Ionization: Where We Stand Now and Go from Here, *A314* 12. The Proteomics Standards Initiative and ProteomeXchange: Supporting Open Data Practices in Proteomics, *A315* 13. Fundamentals: Structural Elucidation of Proteins (Fundamentals Interest Group), *A316* 14. Education: Teaching MS at the Undergraduate Level (Undergraduate Research in MS Interest Group), *A303* 15. New Ion Manipulations Prior to FT-MS (FTMS Interest Group), *A302* 16. Cannabis and Hemp Testing Requirements: How to Leverage with Mass Spectrometry, *A301* 17. Getting Started with R for Mass Spectrometry Data Analysis, *A305* 18. Career and Collaboration Opportunities in China, *A304*
7:00 - 8:00 PM	**DINNER BREAK**
AFTER 8:00 PM	**CORPORATE HOSPITALITY SUITES,** Omni CNN Center Hotel

THURSDAY

7:00 AM	**CORPORATE BREAKFAST SEMINARS,** Convention Center
7:30 AM - 5:00 PM	**REGISTRATION,** Building B Main Lobby
8:30 - 10:30 AM	**ORAL SESSIONS** ThOA am: Informatics: Metabolomics, *Murphy Ballroom, Bldg. B, Level Five* ThOB am: Fundamentals: Ion Spectroscopy, *B401-402* ThOC am: Post-Translational Modifications: Qualitative and Quantitative Analysis, *B405-407* ThOD am: Drug Discovery and Development: Quantitative Analysis, *B302-305* ThOE am: Supramolecular and Macromolecular Complexes, *B308-309* ThOF am: Clinical Analysis Using MS, *B312-314* ThOG am: Informatics: Stable Isotope Labeling in MS: Applications, *Auditorium, Bldg. A* ThOH am: Exposomics, Toxicology, and Human Health, *A411-412*
10:30 AM - 2:30 PM	**POSTER SESSION AND EXHIBITS,** Thursday Posters, Poster/Exhibit Hall ground level **Odd-number posters present:** 10:30 - 11:30 am PLUS 12:30 – 2:30 pm **Even-number posters present:** 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm
2:30 - 4:30 PM	**ORAL SESSIONS** ThOA pm: Informatics: Peptide and Protein Identification, Proteomics, *Murphy Ballroom, Bldg. B* ThOB pm: Microorganisms and the Microbiome, *B401-402* ThOC pm: Quantitative Proteomics in Systems Biology, *B405-407* ThOD pm: Covalent Labeling and Chemical Crosslinking, *B302-305* ThOE pm: Plant "omics", *B308-309* ThOF pm: Ion Mobility: Structure, *B312-314* ThOG pm: Instrumentation: Innovations in Mass Analyzers, *Auditorium, Bldg. A* ThOH pm: Fundamentals: Ion Activation and Dissociation, *A411-412*
4:45 - 5:30 PM	**PLENARY LECTURE,** Murphy Ballroom, Bldg. B, Level Five  **Chemistry of Food and Soft Drinks** **Lilly D'Angelo** *Global Food & Beverage Technology Associates*
6:30 - 9:00 PM	**CLOSING EVENT** **Georgia Aquarium.** *Tickets ($40) must be purchased in advance by Monday 12 noon.* Join us for an enchanting evening at the Georgia Aquarium. Dinner buffets close at 8:00 pm, dessert available until close. Ticket includes aquarium entry for our private event, dinner buffet and one drink ticket for soda, beer, or wine. Cash bars available until close 



SUNDAY EVENING, 4:00 - 9:00 PM

4:00-4:45 pm Sunday
Attention First-time Graduate Students and Undergrads
Plan your Strategy: What to See and Do at ASMS
B302-305 Level Three

5:00-6:30 pm Sunday
TUTORIAL SESSION I
Presiding: Susan Richardson (University of South Carolina)
Murphy Ballroom, Bldg B, Level Five




5:00-5:45 pm
Lipidomics

Stephen Blanksby
Queensland University of Technology
& Gavin Reid
University of Melbourne



5:45-6:30 pm
Targeted Imaging

Enrico Davoli
Mario Negri Institute

5:00-6:30 pm Sunday
TUTORIAL SESSION II
Presiding: Erin Baker (North Carolina State University)
B302-305 Level 3



5:00-5:45 pm
Native Mass Spectrometry

Michal Sharon
Weizmann Institute



5:45-6:30 pm
Data Independent Acquisition

Birgit Schilling
The Buck Institute

6:45- 7:45 pm Sunday
CONFERENCE OPENING
Presiding: Susan Richardson (University of South Carolina)
Murphy Ballroom, Bldg B, Level Five

Welcome, Susan Richardson *University of South Carolina*
ASMS Vice President for Programs



7:00-7:45 pm
Transitioning the World Energy for All Purposes to Stable Electricity Powered by 100% Wind, Water, and Sunlight

Mark Z. Jacobson
Stanford University

7:45-9:00 pm Sunday
WELCOME RECEPTION
Poster/Exhibit Hall (Level One)
Conference name badge is required.



MONDAY MORNING ORAL SESSIONS

From 7:00 am Monday
CORPORATE BREAKFAST SEMINARS
CONVENTION CENTER AND OMNI CNN CENTER HOTEL
See page 16 for detailed schedule. Reservation or RSVP required.

8:30 - 10:30 am Monday
CANNABIS TESTING
Session Chair: Jack Henion (Advion, Inc.)
Murphy Ballroom, Bldg B, Level 5

MOA am 08:30 **Future Opportunities and Challenges in Mass Spectrometry Based Cannabis Analytical QC Testing and Research**; Scott Kuzdzal, Ph.D. [1]; Andrew P. Fornadel, Ph.D. [1]; Jeff H. Dahl, Ph.D. [1]; Bob H. Clifford, Ph.D. [1]; Nicole H. Lock[1]; [1]*Shimadzu Scientific Instruments, Inc., Columbia, MD*

MOA am 08:50 **Novel HR-ESI-LC/MS and SHS-GC-MS/MS Methods for Comprehensive Metabolic Profiling of Phytocannabinoids and Terpenoids in Cannabis**; Paula Berman[1]; Anna Shapira[1]; Ben Yellin[1]; Gil Lewitus[1]; David Meiri[1]; [1]*Technion - Israel Institute of Technology, Haifa, Israel*

MOA am 09:10 **Pesticide Residue Detection in Cannabis and Products using Liquid Chromatography-Mass Spectrometry/Mass Spectrometry (LC-MS/MS)**; Caley B Craven[1]; Ping Jiang[1]; Charles A. Lucy[1]; Xing-Fang Li[1]; [1]*University of Alberta, Edmonton, Alberta*

MOA am 09:30 **Cannabis Testing: Development, Validation, and Implementation of a Patient-centric Microsampling Assay for Analysis of Cannabinoids in Human Whole Blood**; Ganesh Moorthy; *The Children's Hospital of Philadelphia, Philadelphia, PA*

MOA am 09:50 **The Use of Mass Spectrometry for Quality Control and Understanding the Complex Chemistry of Cannabis and Its Therapeutic Effects**; Kaveh Kahen; *Sigma Analytical Services, Toronto, ON*

MOA am 10:10 **Specializing Cannabis Cultivation Quality Control with a Mobile Mass Spectrometry Lab**; Brigitte Simons[1]; Afsoon Pajand Birjandi[1]; Hesham Ghobarah[2]; Ping Jiang[3]; Hubert Marceau[4]; Alexis St-Gelais[4]; Tariq Akhtar[5]; Xing-Fang Li[3]; *[1]Molecular Science Corp., Toronto, ON; [2]Deep Dive Research Inc., Toronto, ON; [3]University of Alberta, Edmonton, AB; [4]Laboratoire PhytoChemia, Chicoutimi, QC; [5]University of Guelph, Guelph, ON*

8:30 - 10:30 am Monday
GLYCOPEPTIDES AND GLYCOPROTEINS
Session Chair: Shujuan McDonald (Pfizer Inc.)
B401-402

MOB am 08:30 **Cost-Benefit Analysis of Stepped-Energy Collisional Dissociation and Electron Transfer Dissociation Approaches for Intact Glycopeptide Characterization**; Nicholas M Riley[1]; Stacy A Malaker[1]; Marc D Driessen[1]; Carolyn R Bertozzi[1]; *[1]Stanford University, Stanford, CA*

MOB am 08:50 **Finding the Sweetspot of Prostate-Specific Antigen**; Guinevere S.M. Lageveen-Kammeijer[1]; Alan B. Moran[1]; Jan Nouta[1]; Elena Dominguez-Vega[1]; Manfred Wuhrer[1]; *[1]Leiden University Medical Center (LUMC), Leiden, Netherlands*

MOB am 09:10 **Advanced Data Acquisition and Processing Approach Increases Glycopeptide Identifications and Improves Confidence of Assignment**; Kevin Brown Chandler[1]; Deborah R Leon[1]; Catherine E Costello[1]; *[1]Department of Biochemistry, Boston University School of Medicine, Boston, MA*

MOB am 09:30 **Large Scale Human Glycoproteomics: Insights into Data Analysis**; Kathleen T. Grassmyer[1]; Christopher J. Brown[1]; Matthew L. MacDonald[2]; David E. Clemmer[1]; Jonathan C. Trinidad[1]; *[1]Indiana University Bloomington, Bloomington, IN; [2]University of Pittsburgh School of Medicine, Pittsburgh, PA*

MOB am 09:50 **Absolute Quantitation of the N-Linked Glycoforms of a Biotherapeutic IgG in Complex Mixtures by HILIC-MRM with an Isotopically Labeled Standard**; Ron Orlando[1, 2]; Marla Popov[2]; Stuart Haslam[3]; Tyler Fletcher[1]; *[1]University of Georgia, Athens, GA; [2]Glycoscientific LLC, Athens, GA; [3]Imperial College, London, United Kingdom*

MOB am 10:10 **Native Mass Spectrometry Analysis of Glycoprotein-Protein/Ligand Interactions**; Di Wu[1]; Carol V. Robinson[1]; *[1]University of Oxford, Oxford, United Kingdom*

8:30 - 10:30 am Monday
MEMBRANE PROTEIN MS
Session Chair: Julien Marcoux (CNRS)
B405-407

MOC am 08:30 **Lipid-Composition Alters Protein Dynamics of Aquaporin Z Nanodisc**; Xin Shan Lim[1]; Xin-Xiang Lim[1]; Lili Wang[1]; Qingsong Lin[1]; Ganesh S Anand[1]; *[1]National University of Singapore, Singapore*

MOC am 08:50 **Detergent- and Chemical-Free Native Mass Spectrometry Reveals the Membrane Protein Complex Ensemble of Whole Membrane Fractions**; Dror Shlomo Chorev[1]; Haiping Tang[1]; Tom Durrant[1]; Siyun Chen[1]; Carol V. Robinson[1]; *[1]University of Oxford, Oxford, United Kingdom*

MOC am 09:10 **Revealing the Structural and Functional Environment of Sialylated Proteins on Cell Surfaces by Quantitative Oxidation Mapping**; Qiongyu Li[1]; Yixuan (Axe) Xie[1]; Gege Xu[1]; Carlito B Lebrilla[1]; *[1]University of California, Davis, CA*

MOC am 09:30 **Localization and Activity of the Metal Centers of Membrane Complexes Using Micelles and Nanodiscs Coupled with Native Top-Down Mass Spectrometry**; Luis F. Schachner[1]; Soo Y Roo[1]; Christopher W Koo[1]; Amy C Rosenzweig[1]; Neil L Kelleher[1]; *[1]Northwestern University, Evanston, IL*

MOC am 09:50 **CellSurfer: An N-Glycoprotein-specific Analysis Platform for Semi-automated, Quantitative Discovery of Cell Surface Proteins**; Amanda Rae Buchberger[1]; Linda Berg Luecke[1]; Rachel A. Jones Lipinski[1]; Ranjuna Weerasekera[1]; Matthew Waas[1]; Rebekah L. Gundry[1]; *[1]Medical College of Wisconsin, Milwaukee, WI*

MOC am 10:10 **Cytochrome P450s Captured within Lipid Nanodiscs Reveal Ligand-dependent Shifts in Gas-phase Stability**; Kristine F Parson[1]; Colleen M. Riordan[1]; Kathrine Gentry[1]; Carlo Barnaba[1, 2]; Ayyalusamy Ramamoorthy[1]; Ryan C. Bailey[1]; Brandon T. Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI; [2]Michigan State University, East Lansing, MI*

8:30 - 10:30 am Monday
IMAGING: INSTRUMENTATION & METHOD DEVELOPMENT
Session Chair: Martina Marchetti-Deschmann (TU Wien)
B302-305

MOD am 08:30 **SPICing up your MALDI Image: Enhanced Ion Yields for Numerous Classes of Lipids via Single-Photon-Induced Chemical Ionization**; Christoph H. M. Bookmeyer[1]; Jens Soltwisch[1, 2]; Ulrich Röhling[3]; Klaus Dreisewerd[1, 2]; *[1]Institute for Hygiene, University of Münster, Münster, Germany; [2]Interdisciplinary Center for Clinical Research (IZKF), University of Münster, Münster, Germany; [3]Institute of Medical Physics and Biophysics, University of Münster, Münster, Germany*

MOD am 08:50 **Identification of Phosphatidylcholine Lipids in Imaging Mass Spectrometry Using Gas-Phase Charge Inversion Ion/Ion Reactions Enabled on an FT-ICR Mass Spectrometer**; Jonathan T Specker[1]; Steve L. Van Orden[2]; Boone M. Prentice[1]; *[1]Department of Chemistry, University of Florida, Gainesville, FL; [2]Bruker Daltonics Inc., Billerica, MA*

MOD am 09:10 **Breast Cancer Tumor and Necrosis Associated Peptide and Glycan Co-Localizations in FFPE Tissues by MALDI-FTICR Imaging Mass Spectrometry**; Danielle A Scott[1]; Laura Spruill[1]; Peggi Angel[1]; Richard Drake[1]; *[1]Medical University of South Carolina, Charleston, SC*

MOD am 09:30 **An Integrated Microfluidic Device for High-Resolution Nano-DESI Mass Spectrometry Imaging of Tissue Sections**; Xiangtang Li[1]; Ruichuan Yin[1]; Julia Laskin[1]; *[1]Purdue University, West Lafayette, IN*

MOD am 09:50 **LADI of All Trades: Imaging of Small-Molecule Spatial Distributions in Complex Matrices by a Novel Ambient Ionization Imaging Technique**; Kristen L Fowble[1]; Rabi A Musah[1]; *[1]University at Albany-SUNY, Albany, NY*

MOD am 10:10 **Revealing Isobaric and Isomeric Substructure in Tissue: Advanced Multivariate Analysis for Ion Mobility Imaging Mass Spectrometry**; Raf Van de Plas[1, 2, 3]; Lukasz Migas[1]; Nathan Heath Patterson[2, 3]; Katerina V. Djambazova[2, 4]; Richard M. Caprioli[2, 3, 4, 5, 6]; Jeffrey M. Spraggins[2, 3, 4]; *[1]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [2]Mass Spectrometry Research Center,*

Vanderbilt University, Nashville, TN; [3]Department of Biochemistry, Vanderbilt University, Nashville, TN; [4]Department of Chemistry, Vanderbilt University, Nashville, TN; [5]Department of Pharmacology, Vanderbilt University, Nashville, TN; [6]Department of Medicine, Vanderbilt University, Nashville, TN

8:30 - 10:30 am Monday
LIPIDOMICS: TARGETED AND UNTARGETED
Session Chair: Peggi Angel
(Medical University of South Carolina)
B308-309

MOE am 08:30 **A 'Systems-omics' Strategy to Uncover the Role of Brain Tissue Derived Exosomal Lipids in Alzheimer's Disease**; Huaqi (Kate) Su[1,2]; Kevin J. Barnham[1,2]; Laura J. Vella[1]; Gavin E Reid[2]; *[1]Florey Institute of Neuroscience and Mental Health, Parkville, Australia; [2]University of Melbourne, Parkville, Australia*

MOE am 08:50 **Comprehensive Phospholipid Analysis Reveals Alternations in Extracellular Vesicles during Immune Responses**; Wenpeng Zhang[1,2]; Ying Zhang[3]; Jiaqi Liang[1]; Bing Shang[1]; Hang Yin[3]; Yu Xia[1,2]; *[1]Department of Chemistry, Tsinghua University, Beijing, China; [2]Department of Chemistry, Purdue University, West Lafayette, IN; [3]School of Pharmaceutical Sciences, Tsinghua University, Beijing, China*

MOE am 09:10 **Localizing the Inflammatory Lipid Response to Structurally Engineered Lipopolysaccharide in Mouse Lung**; Alison J Scott[1,2]; Shane R. Ellis[2]; Courtney E. Chandler[1]; Sung Hwan Yoon[3]; Benjamin L Oyler[4]; David Robinson Goodlett[1]; Ron M. A. Heeren[2]; Robert K. Ernst[1]; *[1]University of Maryland, Baltimore, Baltimore, MD; [2]Maastricht Multimodal Molecular Imaging (M4I) Institute, Division of Imaging Mass Spectrometry, Maastricht, Netherlands; [3]University of Maryland Baltimore, Baltimore, MD; [4]Center for Food Safety and Applied Nutrition, FDA, Silver Spring, MD*

MOE am 09:30 **Next-Generation Imaging Technologies for 3-D Multimodal Lipid Atlases**; Jeffrey M Spraggins[1,2,3]; Nathan Heath Patterson[1,2]; David M. Anderson[1,2]; Jamie Allen[1,2]; William J. Perry[1,2]; Martin Dufresne[1,2]; Lukasz Migas[4]; Danielle Gutierrez[1,2]; Eric P. Skaar[5]; Richard M. Caprioli[1,2,3]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Vanderbilt University Department of Biochemistry, Nashville, TN; [3]Vanderbilt University Department of Chemistry, Nashville, TN; [4]Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands; [5]Vanderbilt University Medical Center Department of Pathology, Microbiology and Immunology, Nashville, TN*

MOE am 09:50 **Integrated Multidimensional Liquid Chromatography-Ion Mobility-Tandem Mass Spectrometry (LC-IM-MS/MS) Workflow for High Confidence Annotations in Global Untargeted Lipidomics**; Bailey S. Rose[1]; Simona G. Codreanu[1]; Jody C. May[1]; Stacy D. Sherrod[1]; John A. McLean[1]; *[1]Vanderbilt University, Nashville, TN*

MOE am 10:10 **In-Depth Lipidomic Profiling of the Australian Imaging Biomarker and Lifestyle Flagship Study of Aging**; Kevin Huynh[1]; Wei Ling Florence Lim[2,3]; Corey Giles[4]; Kaushala S Jayawardana[4]; Pratishtha Chatterjee[2,5,6]; Natalie A Mellett[4]; Ian Martins[2,3]; Simon M Laws[3,7,8]; Ashley I Bush[9]; Christopher C Rowe[9,10]; Victor L Villemagne[9,10,11]; David Ames[12]; Colin L Masters[9]; Brian G Drew[1]; Ralph N Martins[2,3,5,6,13,14]; Peter J Meikle[1,15]; *[1]Baker Heart and Diabetes Institute, Melbourne, Australia; [2]School of Medical and Health Sciences, Edith Cowan University, Perth, Australia; [3]Cooperative Research Centre (CRC) for Mental Health, Perth, Australia; [4]Baker Heart and Diabetes Institute, Melbourne, Australia; [5]Department of Biomedical Sciences, Macquarie University, Sydney, Australia; [6]KaRa Institute of Neurological Disease, Sydney, Macquarie Park, Sydney, Australia; [7]Collaborative Genomics Group, School of Medical and Health Sciences, Edith Cowan University, Perth, Australia; [8]School of Pharmacy and Biomedical Sciences, Faculty of Health Sciences, Curtin Health Innovation, Perth, Australia; [9]Florey Department, University of Melbourne, Melbourne, Australia; [10]Department of Nuclear Medicine and Centre for PET, Austin Health, Melbourne, Australia; [11]Department of Medicine, Austin Health, The University of Melbourne, Melbourne, Australia; [12]National Ageing Research Institute, Parkville, Victoria, Australia; [13]School of Psychiatry and Clinical Neurosciences, The University of Western Australia, Perth, Australia; [14]Australian Alzheimer's Research Foundation, Nedlands, Perth, Australia; [15]Monash University, Melbourne, Australia*

8:30 - 10:30 am Monday
FUNDAMENTALS: ION MOBILITY AND MS
(IN MEMORY OF AL YERGEY)
Session Chair: Stephanie Cologna
(University of Illinois at Chicago)
B312-314

MOF am 08:30 **Ultrahigh Resolution Ion Mobility Separations of Isotopologues and Isotopomers in Multi-Pass Traveling Wave-Based Structures Lossless Ion Manipulations (SLIM)**; Roza Wojcik[1]; Gabe Nagy[1]; Isaac K Attah[1]; Sandilya V.B. Garimella[1]; Yehia M Ibrahim[1]; Richard D. Smith[1]; *[1]PNNL, Richland, WA*

MOF am 08:50 **Fundamental Principles and Experimental Performance of a Novel Counter Flow Ion Mobility Device: U-Shaped Mobility Analyzer**; Keke Wang[1]; Qiao Jin[1]; Xu Zhou[1]; Lin Liu[1]; Kent J. Gillig[2]; Xiaoqiang Zhang[1]; Lei Wang[3]; Yilong Guo[3]; Wenjian Sun[1]; *[1]Shimadzu Research laboratory (Shanghai) Co. Ltd., Shanghai, China; [2]Genomics Research Center, Academia Sinica, Taipei, Taiwan; [3]Shanghai Institute of Organic Chemistry, Chinese Academy of Science, Shanghai, China*

MOF am 09:10 **Maximizing Signal to Noise Ratio for Voltage Sweep Multiplexing-Ion Mobility-Ion Trap Mass Spectrometry**; Tobias Reinecke[1]; Pearl Kwantwi-Barima[1]; Brian H. Clowers[1]; *[1]Department of Chemistry, Washington State University, Pullman, WA*

MOF am 09:30 **Collision Cross Sections of Phosphoric Acid Cluster Anions and their Use as Calibrants for Traveling Wave Ion Mobility**; Valentina Calabrese[1]; Helene Lavanant[1]; Frédéric Rosu[2]; Valérie Gabelica[3]; Carlos Afonso[1]; *[1]Normandie Univ, INSA Rouen, UNIROUEN, CNRS, COBRA, Rouen, France; [2]CNRS, UMS 3033, Institut Européen de Chimie et Biologie (IECB), Pessac, France; [3]University of Bordeaux, INSERM and CNRS, ARNA Laboratory, IECB, Bordeaux, France*

MOF am 09:50 **Combining Direct Metalation and Collision-Induced Unfolding Reveals Structure Changes of Metallothioneins During Ag+ Metalation**; Shiyu Dong[1]; David H. Russell[1]; *[1]Texas A&M University, College Station, TX*

MOF am 10:10 **Advanced Temporal Multiplexing and Peak Deconvolution for Improved Sensitivity and Resolution in Ion Mobility-Mass Spectrometry Analysis**; Jody C. May[1]; Richard Knochenmuss[2]; John C. Fjeldsted[3]; John A. McLean[1]; *[1]Vanderbilt University, Nashville, TN; [2]RKResearch, Seftigen, Switzerland; [3]Agilent Technologies, Santa Clara, CA*

8:30 - 10:30 am Monday
INSTRUMENTATION: PORTABLE AND TRANSPORTABLE MASS SPECTROMETERS
Session Chair: Essyllt Louarn (Université Paris-Sud)
Auditorium, Bldg A

MOG am 08:30 **Miniature OzID Mass Spectrometer for Clinical Lipid Analysis**; Xinwei Liu[1]; Wenbo Cao[2]; Xiaoxiao Ma[2]; Wenpeng Zhang[3]; Stephen J. Blanksby[1]; Yu Xia[3, 5]; Zheng Ouyang[3, 6]; *[1]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instruments, Tsinghua University, Beijing, China; [2]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instruments, Tsinghua University, Bejing, China; [3]Department of Chemistry, Purdue University, West Lafayette, IN 47907; [4]Central Analytical Research Facility, Queensland University of Technology, Brisbane, Australia; [5]Department of Chemistry, Tsinghua University, Beijing, China; [6]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instruments, Tsinghua University, Beijing, China*

MOG am 08:50 **MS2field: Automated Real-Time Water Quality Screening with a Transportable LC-HRMS**; Michael Stravs[1]; Nicole Zehethofer[2]; Reto Bolliger[3]; Guenter Boehm[3]; Thomas Moehring[2]; Heinz Singer[1]; Christian Stamm[1]; Christoph Ort[1]; *[1]Eawag, Duebendorf, Switzerland; [2]Thermo Fisher Scientific, Bremen, Germany; [3]CTC Analytics AG, Zwingen, Switzerland*

MOG am 09:10 **Pulse-sampling Assisted Flash Heating Desorption Miniature Ion Trap Mass Spectrometry with Photoionization for Sensitivity and On-Site Identification of Illegal Drugs**; Keyong Hou[1]; shuang Wang[1]; Weimin Wang[1]; Haiyang Li[1]; *[1]Dalian Institute of Chemical Physics, Chinese Academy of Science, Dalian, China*

MOG am 09:30 **Development and Validation of a Simple Headspace Needle-Trap Method for Quantitative Estimation of Butylated Hydroxyltoluene from Cosmetic by Hand-Portable GC/MS**; Chiranjit Ghosh[1]; Jonathan Grandy[1]; Varoon Singh[1]; Janusz Pawliszyn[1]; *[1]University of Waterloo, Waterloo, ON*

MOG am 09:50 **Designing a Magnetic Sector for a Cycloidal Mass Analyzer in a Miniature Mass Spectrometer**; Kathleen L Horvath[1]; Tanouir Aloui[1]; Raul Vyas[1]; Maria Luisa Sartorelli[1]; Yuriy Zhilichev[2]; Roger P Sperline[3]; M Bonner Denton[3]; Patrick Keelan[4]; David Koester[1]; Jeffrey T Glass[1]; Jason J Amsden[1]; Jesko A von Windheim[1]; *[1]Duke University, Durham, NC; [2]Independent, Durham, NC; [3]University of Arizona, Tucson, AZ; [4]PFT Technology, Long Island, NY*

MOG am 10:10 **Demonstration and Verification of the Pyrolysis and Derivatization GCMS Capabilities of the Mars Organic Molecule Analyzer (MOMA) Mass Spectrometer**; Desmond A. Kaplan[1, 2]; Melissa Guzman[3]; Fabien Stalport[4]; Noel Grande[4]; Cyril Szopa[3, 5]; Caroline Freissinet[6]; Arnaud Buch[7]; Andrej Grubisic[2]; Ryan M. Danell[2, 8]; Friso Van Amerom[9]; Xiang Li[2, 10]; Stephanie A. Getty[2]; William B. Brinckerhoff[2]; Paul R. Mahaffy[2]; *[1]KapScience LLC, Tewksbury, MA; [2]NASA Goddard Space Flight Center, Greenbelt, MD; [3]LATMOS/ IPSL, Université Versailles St Quentin, UPMC Université Paris 06, CNRS, Guyancourt, France; [4]Laboratoire Interuniversitaire des Systèmes Atmosphériques (LISA), Paris, France; [5]Institut Universitaire de France, Paris, France; [6]LATMOS/ IPSL, UVSQ Université Paris-Saclay, Paris, France; [7]CentraleSupelec, Paris, France; [8]Danell Consulting, Inc., Winterville, NC; [9]Mini-Mass Consulting, Inc, Hyattsville, MD; [10]University of Maryland, College Park, MD*

8:30 - 10:30 am Monday
BIOMARKERS: QUALITATIVE ANALYSIS
Session Chair: Jason Hogan (Bristol-Myers Squibb)
A411-412

MOH am 08:30 **Proteomic Assessment of Synapses with Rich Associated Clinical Data Highlight Potential Targets for Mediating Alzheimer's Pathology and Cognitive Decline**; Becky C Carlyle[1, 2]; Savannah E. Kandigian[1]; Bianca A. Trombetta[1]; Wilhelm Haas[1, 2]; Steven E. Arnold[1, 2]; *[1]Massachusetts General Hospital, Charlestown, MA; [2]Harvard Medical School, Boston, MA*

MOH am 08:50 **Proteome Profiling of Multiple Sclerosis Cerebrospinal Fluid by Data Independent Acquisition Reveals Disease Biomarkers**; David R. Spiciarich[1]; Christopher T. Harp[1]; Ann E. Herman[1]; W. Rodney Mathews[1]; Veronica G. Anania[1]; *[1]Genentech, Inc., South San Francisco, CA*

MOH am 09:10 **Urine Metabolomics of Children with Autism Spectrum Disorder (ASD) Treated with Sulforaphane**; Roshanak Aslebagh[1]; Kanwaljit Singh[2]; Michelle L. Dubuke[1]; Andrew W. Zimmerman[2]; Scott A. Shaffer[1]; *[1]Department of Biochemistry and Molecular Pharmacology, University of Massachusetts Medical School, Worcester, MA; [2]Department of Pediatrics (Neurology), University of Massachusetts Medical School, Worcester, MA*

MOH am 09:30 **Unraveling a Complex Immunoprotein Profile in Multiple Myeloma with Middle-Down *de novo* Sequencing and Native Mass Spectrometry**; Valerie J Winton[1, 2]; W Ian Deighan[3]; Lissa C. Anderson[4]; Rafael D. Melani[1, 2]; Luis F. Schachner[1]; Feargal P McNicholl[3]; John P. McGee[1]; Romain Huguet[5]; Philip M Remes[5]; Christopher Mullen[5]; Paul M Thomas[1, 2]; Neil L Kelleher[1, 2]; *[1]Northwestern University, Evanston, IL; [2]Proteomics Center of Excellence, Northwestern University, Chicago, IL; [3]Altnagelvin Hospital, Londonderry, United Kingdom; [4]National High Magnetic Field Laboratory, Tallahassee, FL; [5]Thermo Fisher Scientific, San Jose, CA*

MOH am 09:50 **Proteogenomic Analyses of Peptide Ancestry Informative Markers in Uterine Neoplasms from Women of European, African and Asian Descent**; Nicholas W Bateman[1, 2]; Brian Hood[1]; Christopher Tarney[1]; Michael Kessler[3]; Zhou Ming[4]; Alexander Wong[1]; Anthony R Soltis[5]; Xijun Zhang[5]; Clifton Dalgard[5]; Mathew Wilkerson[5]; Kathleen Darcy[1, 2]; Yovanni Casablanca[1, 2]; George Larry Maxwell[1, 2, 4]; Timothy O'Connor[3]; Thomas P. Conrads[1, 2, 4]; *[1]Gynecologic Cancer Center of Excellence, Annandale, VA; [2]John P. Murtha Cancer Center, Bethesda, MD; [3]Institute for Genome Sciences and the Department of Medicine University of Maryland*

School of Medicine, Baltimore, MD; [4]Inova Schar Cancer Institute, Annandale, VA; [5]The American Genome Center, Uniformed Services University, Bethesda, MD

MOH am 10:10 **BloodKB: An Open Community-Scale Knowledge Base for Blood-Related Proteome and Peptidome Diversity**; Benjamin Pullman[1]; Julie S Wertz[1]; Nuno Bandeira[1]; *[1]University of California, San Diego, La Jolla, CA*

10:30 am-2:30 pm Monday
MONDAY POSTER SESSION
Poster/Exhibit Hall ground level
Lunch concessions are open 11:00 am - 2:00 pm

Odd-number posters present:
10:30 am - 11:30 am PLUS 12:30- 2:30 pm

Even-number posters present:
10:30 am - 12:30 pm PLUS 1:30- 2:30 pm
Poster Pick-Me-Up Snacks served at 1:30 pm

11:30 am - 1:00 pm
Undergraduate Students
"Meet the Experts" at tables reserved for you.

MONDAY AFTERNOON ORAL SESSIONS

2:30 - 4:30 pm Monday
INFORMATICS: MULTIOMICS INTEGRATION AND APPLICATIONS
Session Chair: Ewy Mathe (Ohio State University Medical Center)
Murphy Ballroom, Bldg B, Level 5

MOA pm 02:30 **ProteomicsDB: A Big-Data, Multi-Omics, Multi-Organism Resource for Life Science Research**; Patroklos Samaras[1]; Tobias Schmidt[1]; Pia Bothe[1]; Martin Frejno[1]; Siegfried Gessulat[1,2]; Jana Zecha[1]; Anna Jarzab[1]; Maria Reinecke[1]; Julia Mergner[1]; Piero Giansanti[1]; Johannes Rank[3]; Harald Kienegger[3]; Helmut Krcmar[3]; Hans-Christian Ehrlich[2]; Stephan Aiche[2]; Bernhard Kuster[1,4]; Mathias Wilhelm[1]; *[1]Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; [2]SAP SE, Potsdam, Germany; [3]Chair for Information Systems, Technical University of Munich, Munich, Germany; [4]Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany*

MOA pm 02:50 **Cognitive Re-Analysis of Metabolomics Data Reveals Newly-Associated Metabolite Biological Functions and Mechanistic Predictions of Activity**; Erica Majumder[1]; Elizabeth M Billings[1]; H. Paul Benton[1]; Richard L Martin[2]; Amelia Palermo[1]; Carlos Guijas[1]; Markus M Rinschen[1]; Xavier Domingo-Almenara[1]; J. Rafael Montenegro-Burke[1]; Gary Siuzdak[1]; *[1]The Scripps Research Institute, La Jolla, CA; [2]IBM Watson Health, Cambridge, MA*

MOA pm 03:10 **Data Integration of Proteomics and Metabolomics from Sugarcane Leaves upon Water Deficit**; Ilara Gabriela Frasson Budzinski[1]; Fabricio Edgar de Moraes[1]; Thais Regiani Cataldi[1]; Livia Maria Franceschini[1]; Carlos Alberto Labate[1]; *[1]ESALQ, Piracicaba, Brazil*

MOA pm 03:30 **Linking Cell Lines to Proteotypes: A Proteome-Level Analysis of Protein Interactions, Expression Levels, and Post-Translational Modifications**; Edward L. Huttlin[1]; Raphael J Bruckner[1]; Jose Navarrete-Perea[1]; David Nusinow[1]; Brandon M. Gassaway[1]; Fana Gebreab[1]; Kurt Baltier[1]; Melanie Gygi[1]; Laura Pontano Vaites[1]; Joao A. Paulo[1]; J. Wade Harper[1]; Steve Gygi[1]; *[1]Harvard Medical School, Boston, MA*

MOA pm 03:50 **A Web-based Platform for Data Exploration and Its Application to Multi-omic Profiling of a Large CRISPR Knockout Collection**; Dain Ryan Brademan[1]; Evgenia Shishkova[1]; Jarred Rensvold[2]; Paul D Hutchins[1]; Sean Peters[1]; Adam Jochem[2]; Alexander S. Hebert[1]; Nicholas W Kwiecien[1]; Ian J Miller[1]; Michael S Westphall[1]; David J Pagliarini[2]; Joshua J Coon[2,3,4,5]; *[1]University of Wisconsin - Madison, Madison, WI; [2]Morgridge Institute for Research, Madison, WI; [3]Genome Center of Wisconsin, Madison, WI; [4]Department of Chemistry, University of Wisconsin, Madison, WI; [5]Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI*

MOA pm 04:10 **More Than Just a List: An Accessible and Flexible Informatics Environment for Proteogenomic Data Processing, Interpretation and Hypothesis-Generation**; Timothy J. Griffin[1]; Praveen Kumar[1,2]; James E. Johnson[3]; Thomas McGowan[3]; Ray W. Sajulga[1]; Subina Mehta[1]; Pratik D. Jagtap[1]; *[1]University of Minnesota, Minneapolis, MN; [2]Bioinformatic and Computational Biology Program, University of Minnesota, Rochester, MN; [3]Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, MN*

2:30 - 4:30 pm Monday
HOMELAND SECURITY: CHEMICAL/BIOLOGICAL DEFENSE
Session Chair: Carolyn Koester
(Lawrence Livermore National Laboratory)
B401-402

MOB pm 02:30 **Infrared Thermal Desorption DART-MS of Trace Explosive Fuel-Oxidizer Mixtures: Powders, Propellants, and Pyrotechnics**; Thomas P. Forbes[1]; Jennifer R. Verkouteren[1]; Edward Sisco[1]; Matthew Staymates[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

MOB pm 02:50 **Screening of Chemical Warfare Agent Simulants and Hydrolysis Products in Soil Using Paper Spray Mass Spectrometry**; Sarah Dowling[1]; Trevor Glaros[2]; Nicholas Manicke[1]; *[1]IUPUI, Indianapolis, IN; [2]ECBC, Aberdeen Proving Ground, MD*

MOB pm 03:10 **Traceable Opioid Material Kits for Mass Spectrometric Opioid Detection in U.S. Laboratories**; Mike A Mojica[1]; Melissa Carter[1]; Samantha L Isenberg[1]; Cody I Sheppard[1]; Elizabeth I. Hamelin[1]; Rebecca L. Shaner[1]; Craig Seymour[1]; Rudolph C. Johnson[1]; *[1]CDC, Atlanta, GA*

MOB pm 03:30 **Mass Spectrometric Detection and Characterization of Botulinum Neurotoxins**; Suzanne R. Kalb[1]; John R. Barr[1]; *[1]CDC, Atlanta, GA*

MOB pm 03:50 **Fast and Efficient Immuno-MALDI Proteomics for Reliable Quantification of Abrin Toxin in Complex Food Matrices**; Sandrine Livet[1]; Sylvia Worbs[2]; Eva Hansbauer[1]; Hervé Volland[3]; Stéphanie

Simon[3]; Christophe Junot[4]; François Fenaille[1]; Brigitte Dorner[2]; Francois Becher[1]; *[1]CEA Saclay, Service de Pharmacologie et Immunoanalyse (SPI) - Laboratoire d'Etude du Métabolisme des Médicaments, Gif-Sur-Yvette, France; [2]Robert Koch Institute, Biological Toxins - Centre for Biological Threats and Special Pathogens, Berlin, Germany; [3]CEA Saclay, Service de Pharmacologie et Immunoanalyse (SPI) - Laboratoire d'Etude et de Recherche en Immunoanalyse, Gif Sur Yvette, France; [4]CEA Saclay, Service de Pharmacologie et Immunoanalyse (SPI), Gif Sur Yvette, France*

MOB pm 04:10 **Highly Accurate Classification of Biological Spores by Culture Medium for Forensic Attribution Using Multiple Chemical Signature Types and Machine Learning**; Paul J. Ippoliti[1]; Michael Crenshaw[1]; Michael Sworin[1]; Frances E. Nargi[1]; Tara L. Boettcher[1]; Matthew E. Walsh[1]; Amanda M. Casale[1]; Jason J. Han[1]; Joshua R. Dettman[1]; *[1]MIT Lincoln Laboratory, Lexington, MA*

2:30 - 4:30 pm Monday
FOOD SAFETY & CHEMISTRY: FOODOMICS, ALLERGENS, BACTERIA, FOODS, AND SUPPLEMENTS
Session Chair: Michelle Colgrave (CSIRO)
B405-407

MOC pm 02:30 **Towards a Proper Drop Time for Coffee Beans during Roasting with Maximized Antioxidant Capacity Using Photoionization Mass Spectrometry**; Jan Heide[1]; Hendryk Czech[1]; Patrick Martens[1]; Michael Wendler[1]; Sven Ehlert[1]; Andreas Walte[2]; Ralf Zimmermann[1]; *[1]University of Rostock, Rostock, Germany; [2]Photonion GmbH, Schwerin, Germany*

MOC pm 02:50 **A PRM-based MS Method for Detection of Milk-Derived Ingredients from a Processed Food Matrix**; Bini Ramachandran[1]; Shyamali Jayasena[1]; Charles T Yang[2]; Melanie Downs[1]; *[1]Food Allergen Research and Resource Program, University of Nebraska, Lincoln, NE; [2]Thermo Fisher Scientific, San Jose, CA*

MOC pm 03:10 **Development of an Encyclopedia of Food Carbohydrates: A Rapid-Throughput LC-MS Based Approach to Global Carbohydrate Analysis of 1000 Foods**; Matthew Amicucci[1]; Eshani Nandita[1]; Ace G. Galermo[2]; Thai-Thanh T Vo[2]; Megan Lee[2]; Carlito B Lebrilla[2]; Yiyun Liu[2]; *[1]University of California Davis, CA; [2]University of California, Davis, CA*

MOC pm 03:30 **A Novel Dereplication Strategy for Comprehensive Studying the Unique Composition of Saponins in Taiwan Quinoa Using High-Resolution Mass Spectrometry**; Hong-jhang Chen[1]; Gui-ru Xie[1]; *[1]National Taiwan University, Taipei, Taiwan*

MOC pm 03:50 **A Novel, Step-Wise Nutrimetabolomics Approach Reveals Small Molecule-Associated Changes in a DASH-Diet Study**; Nichole Reisdorph[1]; Minghua Tang[1]; Audrey Hendricks[1]; Katrina Doenges[1]; Richard Reisdorph[1]; Brian Tooker[1]; Kevin Quinn[1]; Wayne Campbell[2]; Nancy Krebs[1]; *[1]University of Colorado Anschutz Medical Campus, Aurora, CO; [2]Purdue University, West Lafayette, IN*

MOC pm 04:10 **Fast Profiling and Classification of Wines and Wine Quality *via* SAWN-MS**; Alina Astefanei[1]; Roselina Medico[1]; Lauren Pintabona[1]; Petra Jansen[1]; Garry Corthals[1]; *[1]University of Amsterdam, Amsterdam, Netherlands*

2:30 - 4:30 pm Monday
THERAPEUTIC PROTEINS, ANTIBODIES, AND ANTIBODY/DRUG CONJUGATES
Session Chair: Dhanashri Bagal (Amgen)
B302-305

MOD pm 02:30 **Characterizing and Quantitating Biotransformation of Larger Atypical Antibody Therapeutics Using Affinity Capture and SampleStream™ for Intact Protein Mass Spectrometry**; John C. Tran[1]; Hae-Min Park[2]; Wenjing Li[1]; Neha Srikumar[1]; Cong Wu[1]; Phillip Y. Chu[1]; William S. Sawyer[1]; Yichin Liu[1]; Philip D. Compton[3]; *[1]Genentech, South San Francisco, CA; [2]Proteomics Center of Excellence, Northwestern University, Chicago, IL; [3]Integrated Protein Technologies, Inc., Evanston, IL*

MOD pm 02:50 **Discovery of Bioactive Proteins Derived from Scorpion Venom using Two Dimensional Mass Spectrometry**; Meng Li[1]; Pui Yiu Lam[1]; Peng Chen[2]; Remy Gavard[1]; Kung Ching Cookson Chiu[1]; Qiong Wu[2]; Christopher A. Wootton[1]; Mark P. Barrow[1]; Hongzheng Fu[2]; Peter B. O'Connor[1]; *[1]University of Warwick, Coventry, United Kingdom; [2]Peking University, Beijing, China*

MOD pm 03:10 **Intact Protein Mass Spectrometry Guiding Cell Line Development for Tri-specific Antibodies**; Fateme Tousi[1]; Yan Jiang[1]; Susan Elliott[1]; Anthony Paiva[1]; Karen Albee[1]; Karen Lee[1]; *[1]Sanofi, Framingham, MA*

MOD pm 03:30 **Cation-Exchange Chromatography – Mass Spectrometry and Top-Down Analysis of Therapeutic Proteins**; Rachel Liuqing Shi[1]; Gang Xiao[1]; Thomas M Dillon[1]; Margaret S Ricci[1]; Pavel V. Bondarenko[1]; *[1]Amgen, Inc., Thousand Oaks, CA*

MOD pm 03:50 **Direct Determination of Antibody Chain Pairing by Top-Down Mass Spectrometry Using Electron Capture Dissociation and Ultraviolet Photodissociation**; Weijing Liu[1]; Neha Malhan[1]; Yury V. Vasil'ev[2,3]; Joseph S. Beckman[2,3]; Valery G. Voinov[2,3]; Jared B. Shaw[1]; *[1]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA; [2]e-Msion Inc., Corvallis, OR; [3]Linus Pauling Institute, Oregon State University, Corvallis, OR*

MOD pm 04:10 **Collision Induced Unfolding Enables the Rapid Analysis of Stressed Monoclonal Antibodies and Biosimilars**; Daniel D Vallejo[1]; Daniel A. Polasky[1]; Jukyung Kang[2]; Kathryn D. Kulju[1]; Alexander Benet[2]; Ruwan T Kurulugama[3]; John C. Fjeldsted[3]; Anna Schwendeman[2]; Brandon T. Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI; [2]Department of Pharmaceutical Science, University of Michigan, Ann Arbor, MI; [3]Agilent Technologies, Inc., Santa Clara, CA*

2:30 - 4:30 pm Monday
LIPIDOMICS: NEW MS TECHNOLOGIES AND APPLICATIONS
Session Chair: Christina Jones (NIST)
B308-309

MOE pm 02:30 **Quantitative Lipidomics Profiling Reveals Metabolic Subphenotypes in a Cross-Sectional Human Cohort**; Daniel Hornburg[1]; Kevin Contrepois[2]; Sara Ahadi[3]; Kegan Moneghetti[3]; Si Wu[3]; Ming-Shian Tsai[2]; Eric Wei[2]; Jeniffer Quijada[2]; Francois Haddad[2]; Michael Snyder[2]; *[1]Stanford, Palo Alto, CA; [2]Stanford University, Stanford, CA; [3]Stanford University, Palo Alto, CA*

MOE pm 02:50 **Genome-Guided Lipid Identification - A Novel Aid for Hopeless Cases**; Vanessa Linke[1]; Ian J Miller[1,2]; Dain Ryan Brademan[1]; Paul D Hutchins[1]; Edna A Trujillo[1]; Thiru R Reddy[3]; Jason D Russell[3]; Kathryn

L Schueler[1]; Donald S Stapleton[1]; Mary E Rabaglia[1]; Mark P Keller[1]; Daniel M Gatti[4]; Greg Keele[4]; Duy Pham[4]; Gary A Churchill[4]; Alan D Attie[1]; Joshua J Coon[2, 3, 5, 6]; *[1]University of Wisconsin, Madison, WI; [2]Genome Center of Wisconsin, Madison, WI; [3]Morgridge Institute for Research, Madison, WI; [4]The Jackson Laboratory, Bar Harbor, ME; [5]Department of Chemistry, University of Wisconsin, Madison, WI 53706; [6]Department of Biomolecular Chemistry, University of Wisconsin-Madison, WI*

MOE pm 03:10 **Rapid and Simple Differentiation of Lipid Regioisomers in Complex Biological Samples**; Johan Lilja[1]; Kyle D. Duncan[1]; Pontus Gieselsson[2]; Fredrik Palm[1]; Ingela Lanekoff[1]; *[1]Uppsala University, Uppsala, Sweden; [2]Lund University, Lund, Sweden*

MOE pm 03:30 **Conformational Lipid Atlas for High Confidence Lipidomics**; Katrina L. Leaptrot[1]; Jody C. May[1]; James N. Dodds[2]; John A. McLean[1]; *[1]Vanderbilt, Nashville, TN; [2]North Carolina State University, Raleigh, NC*

MOE pm 03:50 **A Novel Solid Phase Sample Preparation Method for Lipidomic Analysis of Plasma Samples**; James A. Apffel[1]; Limian Zhao[2]; Mark Sartain[1]; *[1]Agilent Laboratories, Santa Clara, CA; [2]Agilent Technologies, Wilmington, DE*

MOE pm 04:10 **Laser-Ablation Rapid Evaporative Ionization Mass Spectrometry (LA-REIMS) for Fast Lipidomic Analysis of Genetically Modified CHO Cells in Ambient Conditions**; Stefania Maneta-Stavrakaki[1]; Alvaro Perdones-Montero[1]; Simon Cameron[1]; Julia Abda[1]; Yuen-Ting Chim[2]; Paloma Diaz-Fernandez[2]; Zoltán Takáts[1]; *[1]Imperial College London, London, United Kingdom; [2]GSK, Stevenage, United Kingdom*

2:30 - 4:30 pm Monday
BIOMARKERS: QUANTITATIVE ANALYSIS
Session Chair: Suraj Saraswat (ARUP Lab)
B312-314

MOF pm 02:30 **Targeted Metabolomic Analysis of Urine for Validating Diagnostic Biomarkers of Asthma and COPD**; Mona M. Khamis[1]; Hanan Awad[1]; Darryl J Adamko[2]; Nancy Klemm[3]; Teagan Holt[1]; Mays Al-Dulaymi[4]; Anas El-Aneed[1]; *[1]College of Pharmacy and Nutrition, University of Saskatchewan, Saskatoon, Saskatchewan; [2]2Department of Pediatrics, College of Medicine, Saskatoon, Saskatchewan; [3]Brandenburg University of Technology Cottbus-Senftenberg, Senftenberg, Germany; [4]Department of Pediatrics, College of Medicine, Saskatoon, Saskatchewan*

MOF pm 02:50 **Development and Quantitative Characterization of a Reproducible Method for Proteomic Analysis of Circulating Extracellular Vesicles**; Patrick Vanderboom[1]; Gregory N Ruegsegger[1]; Katherine A Klaus[1]; Dawn M Morse[1]; Surendra Dasari[1]; Ian R Lanza[1]; Sreekumaran Nair[1]; *[1]Mayo Clinic, Rochester, MN*

MOF pm 03:10 **The Role of Mass Spectrometry in Newborn Screening for Krabbe Disease**; Sara E Smith[1]; Jim DiPerna[1]; Melissa Longua[1]; Erica L Fox[1]; *[1]PerkinElmer Genomics, Pittsburgh, PA*

MOF pm 03:30 **An Innovative Multi Point Internal Calibrator (MPIC) Isotopic Dilution Strategy for Biomarker Quantitation by LC-MS/MS**; Shaoxia Yu[1]; Guowen Liu[1]; Thomas Roddy[1]; Max Lein[1]; Dongwei Zhu[1]; Rohini Narayanaswamy[1]; Unnati Kapadnis[1]; Hua Yang[1]; Jose Castro-Perez[1]; *[1]Agios Pharmaceuticals, Cambridge, MA*

MOF pm 03:50 **SASP Atlas: A Database of Senescent Cell Secretomes**; Nathan Basisty[1]; Abhijit Kale[1]; Okhee Jeon[1]; Chisaka Kuehnemann[1]; Therese Payne[1]; Chirag Rao[1]; Anja Holtz[1]; Samah Shah[1]; Judith Campisi[1, 2]; Birgit Schilling[1]; *[1]The Buck Institute for Research on Aging, Novato, CA; [2]Lawrence Berkeley Laboratory, Berkeley, CA*

MOF pm 04:10 **One Injection Does It All: Small Molecule Drug Pharmacokinetics (PK), Drug Metabolites, and Pharmacodynamics (PD) Biomarkers**; Steven Gernhardt[1]; Brendan Tierney[2]; Gang Xing[3]; Amit Kalgutkar[3]; Christopher Holliman[2]; Ragu Ramanathan[2]; *[1]Pfizer, Groton, CT; [2]Pfizer Inc., Groton, CT; [3]Pfizer WRD, Cambridge, MA*

2:30 - 4:30 pm Monday
INSTRUMENTATION: NEW DEVELOPMENTS IN IONIZATION AND SAMPLING
Session Chair: Emmanuelle Claude (Waters Corporation)
Auditorium, Bldg A

MOG pm 02:30 **iTrEnDi on Biomolecules and Beyond: Enhancing MS-Based Quantitative Analyses Using New in Situdiazoalkane Chemistry**; Samuel W Shields[1]; Peter Pallister[1]; Christian Rosales[1]; Carlos R Canez[1, 2]; Karl V Wasslen[1]; John Rivada[1]; Chelsey Aulenback[1]; Joshua Roberts[1]; Fraser Colquhoun[1]; Jeff Manthorpe[1]; Jeffrey C. Smith[1]; *[1]Carleton University, Ottawa, ON; [2]University of Alberta, Edmonton, AB*

MOG pm 02:50 **Integration of a Picodroplet Microfluidic Chip with Mass Spectrometry - A Step towards High Throughput Directed Evolution Screening**; Emily E. Kempa[1]; Clive A. Smith[2]; Xin Li[2]; Perdita E. Barran[1]; *[1]The University of Manchester, Manchester, United Kingdom; [2]Sphere Fluidics Limited, Cambridge, United Kingdom*

MOG pm 03:10 **Deep-ultraviolet Laser Ablation Sampling for Mass Spectrometry**; Remilekun O. Lawal[1]; Fabrizio Donnarumma[1]; Kermit K. Murray[1]; *[1]Louisiana State University, Baton Rouge, LA*

MOG pm 03:30 **Direct Thermal Analysis Methods as Sample Introduction for High-Resolution Mass Spectrometry – Molecular Level Description of Heavy Petroleum Fractions**; Christopher Paul Rüger[1, 2, 3]; Uwe Käfer[2, 4]; Johann Le Maître[3, 5]; Anika Neumann[1, 2]; Oscar Lacroix Andrivet[3]; Marie Hubert-Roux[3]; Benoit Paupy[6]; Sabrina Marceau[5]; Thomas Gröger[1]; Martin Sklorz[2, 4]; Carlos Afonso[3]; Pierre Giusti[5]; Ralf Zimmermann[1, 2, 4]; *[1]University of Rostock, Institute of Chemistry, Division of Analytical and Technical Chemistry, Rostock, Germany; [2]Joint Mass Spectrometry Centre, University of Rostock, Rostock, Germany; [3]Normandy University, COBRA laboratory, Mont Saint Aignan, France; [4]Joint Mass Spectrometry Centre, Comprehensive Molecular Analytics, Helmholtz Zentrum München, Neuherberg, Germany; [5]Total Research & Technology Gonfreville, Harfleur, France*

MOG pm 03:50 **More Inclusive Ionization Demonstrated for Direct Bacteria Differentiation by Combining Automated ESI, MAI, and SAI Methods**; Charles N McEwen[1]; Darrell Marshall[2]; Santosh Karki[2, 3]; Milan Popkristic[2]; Khoa Hoang[1]; Sarah Trimpin[3]; Adetoun Adenijii-Adele[1]; John W Tomsho[1]; *[1]Univ. of the Sciences, Philadelphia, PA; [2]MSTM, LLC, Newark, DE; [3]Wayne State University, Detroit, MI*

MOG pm 04:10 **T-MALDI-2-Orbitrap MS: Sensitive Ion Imaging with Sub-Micrometer Resolution and ppm Mass Accuracy**; Marcel Niehaus[1]; Jens Soltwisch[1, 2]; Mikhail Belov[3]; Klaus Dreisewerd[1, 2]; *[1]Institute of*

Hygiene, University of Münster, Münster, Germany; [2]Interdisciplinary Center for Clinical Research (IZKF), University of Münster, Münster, Germany; [3]Spectroglyph, LLC, Kennewick, WA

2:30 - 4:30 pm Monday
ART, ARCHAEOLOGY, AND PALEONTOLOGY
Session Chair: Julie Arslanoglu
(The Metropolitan Museum of Art)
A411-412

MOH pm 02:30 **New Molecular Evidence of Restoration Treatments Applied to Historic Coptic Manuscripts Using Protein Crosslinking and Top Down Proteomics**; Francesca Galluzzi[1,2]; Catherine M. Rawlins[1,2]; Stéphane Claverol[2]; Federica Pozzi[3]; Maria Fredericks[4]; Franck Trujillo[4]; Caroline Tokarski[1,2]; *[1]Institute of Chemistry and Biology of Membrane and NanoObjects, UMR CNRS 5248, Bordeaux, France; [2]Proteome Platform, Center of Functional Genomics of Bordeaux, University of Bordeaux, Bordeaux, France; [3]Department of Scientific Research, The Metropolitan Museum of Art, New York, NY; [4]Thaw Conservation Center, The Morgan Library & Museum, New York, NY*

MOH pm 02:50 **A Minimally Invasive and Portable Tool for MS Identification of Proteins in Ancient Paintings**; Georgia Ntasi[1]; Paola Cicatiello[1]; Gennaro Marino[1,2]; Paola Giardina[1]; Leila Birolo[1]; *[1]Dept. Chemical Sciences, University of Naples Federico II, Naples, Italy, Naples, Italy; [2]BIOGEM Institute, Ariano Irpino (AV), Italy, Ariano Irpino (AV), Italy*

MOH pm 03:10 **Early Pleistocene (1.8 million years old) Enamel Proteome Sequences Resolve Stephanorhinusphylogeny**; Enrico Cappellini[1]; Frido Welker[1]; Jazmin Ramos Madrigal[1]; Diana Samodova[2]; Patrick L. Ruether[2]; Jesper V. Olsen[2]; David Lordkipanidze[3]; Eske Willerslev[1]; *[1]Natural History Museum of Denmark, Copenhagen, Denmark; [2]NNF Center for Protein Research University of Copenhagen, Copenhagen, Denmark; [3]Georgian National Museum, Tbilisi, Georgia*

MOH pm 03:30 **Single-Pot Solid-Phase-Enhanced Sample Preparation (SP3) for Bone Paleoproteomics**; Timothy Cleland; *Museum Conservation Institute, Smithsonian Institution, Suitland, MD*

MOH pm 03:50 **DeamiDATE 1.0: Site-Specific Deamidation as a Tool to Assess Authenticity of Members of Ancient Proteomes**; Abigail Ramsøe[1,2]; Vivian van Heekeren[1]; Ian Barnes[2]; Camilla Speller[3]; Matthew J Collins[4,5]; *[1]BioArCh, Department of Archaeology, University of York, York, United Kingdom; [2]Department of Earth Sciences, Natural History Museum, London, United Kingdom; [3]Department of Anthropology, University of British Columbia, Vancouver, BC; [4]EvoGenomics Section, Natural History Museum of Denmark, University of Copenhagen, Copenhagen, Denmark; [5]McDonald Institute for Archaeological Research, Downing St, Cambridge, United Kingdom*

MOH pm 04:10 **A Proteomic Workflow to Extract, Concentrate, Digest, and Enrich Peptides from Fossils with High Humic Content for Mass Spectrometry Analyses**; Elena R. Schroeter[1]; Kevin Blackburn[2]; Michael B. Goshe[1]; Mary H. Schweitzer[1]; *[1]North Carolina State University, Raleigh, NC; [2]Waters Corporation, Milford, MA*

4:45-5:30 pm Monday
AWARD LECTURE
Richard A. Yost (University of Florida), presiding
Murphy Ballroom, Bldg B, Level 5

Presentation of the Al Yergey MS Scientist Award
Jeffrey Shabanowitz, *University of Virginia*



John B. Fenn Award for a Distinguished Contribution in Mass Spectrometry

John R. Yates III
The Scripps Research Center

5:45 - 7:00 PM MONDAY WORKSHOPS

There will be light refreshments in Building A foyers. All workshops are in Building A.

01 High Spatial Resolution 2D and 3D Mass Spectrometry Analysis: Current Trends
Presiding: Francisco Fernandez-Lima, Christopher Anderson, Gregory Fisher
A402-403

Advances on 2D and 3D Mass Spectrometry analysis currently drive research in biological, biomedical, materials, environmental and forensic sciences. With the development of new and the incorporation of hyphenated techniques during 2D and 3D MS analysis, the MS community needs to further develop universal analysis and data processing protocols; definitions; reference guidelines; standard reference materials; and inter-laboratory comparisons.

In this third workshop, we will provide a short overview of the state of the art from experts in the field and provide ample time for discussion focused on the definitions of and protocols for testing performance metrics; strategies for sample preparation; data analysis, data processing and data reporting workflows.

A preliminary list of topics will include:
i) Fundamentals of high spatial resolution in 2D and 3D MS analysis (tutorial)
ii) Overview of current and new imaging modalities: challenges and perspectives
iii) Influence of instrument settings and use of standards for 2D and 3D MS imaging
iv) 2D and 3D MS imaging data in public repositories: vendor and user's perspectives

The workshop encourages the participation and presentations of new investigators, postdocs and graduate students. A combination of short presentations (2-3 slides/group) from representatives of the 2D and 3D MS imaging techniques, with a balance between academic, national laboratories and industrial researchers will be followed by an open discussion forum. One of the goals of this workshop is to gather researchers and enable the discussion towards the development of an interest group within the ASMS community to address these new scientific challenges.



5:45 - 7:00 PM MONDAY WORKSHOPS

There will be light refreshments in Building A foyers. All workshops are in Building A.

02 Enhancing MS-Based Glycomics and Glycoproteomics Toolbox: Round-table Discussion
Presiding: Yehia Mechref
A404-405

Glycosylation is a prevalent posttranslational modification of proteins in mammalian cells. Many proteins act through oligosaccharide recognition. Glycosylation of proteins is one of the most common protein posttranslational modifications. The glycans of the membrane or secreted glycoproteins are responsible for modulating and controlling many of the biological roles of these glycoproteins, including cell signaling, adhesion, and communication. Protein folding, stability, and localization are dependent on protein glycosylation. A correlation between changes in the glycans of glycoproteins and many mammalian diseases, such as hereditary disorders, immune deficiencies, cardiovascular disease, and cancer has been, suggested. This and the biological roles of glycans have created a demand for reliable glycomics and glycoproteomics strategies, permitting sensitive monitoring of glycans in biological systems. Mass spectrometry-based glycomics and glycoproteomics methods, glycan and glycoproteins standards and bioinformatics tools are continuously being introduced. However, glycomics and glycoproteomics strategies are far from being routing or automated as proteomics strategies. This workshop will focus on discussing and highlighting what needs to be done to attain complete automation of glycomics and glycoproteomics analyses. The workshop will have a roundtable format and will not include any presentations. The workshop will be addressing questions to be solicited from glycomics and glycoproteomics experts in advance of the meeting, including but not limited to, what is hindering the automation of glycome and glycoproteome analysis, why are glycomics and glycoproteomics strategies not as routinely used as proteomics strategies, how can we overcome the lack of reliable standards, and why a uniform bioinformatics tools are lacking.

03 MassIVE Translation of Public Mass Spectrometry Big Data into Reusable Community Resources
Presiding: Nuno Bandeira, Mingxun Wang
A406-407

The productive reutilization of the very large volumes of public proteomics and metabolomics mass spectrometry data continues to be hindered by significant challenges in the limited findability, accessibility and integration of datasets and reanalysis results. This workshop will focus on approaches addressing these challenges by i) systematically reanalyzing public data using open-source advanced algorithms, ii) reorganizing reanalysis results into open community-scale knowledge bases, and iii) integrating global results into freely-accessible data analysis workflows available free of charge to all research labs.

This workshop is designed to be highly interactive and will aim to inform as well as to promote discussion about ways in which public mass spectrometry big data can be made most useful for the community as a whole.

04 Mass Spectrometry in the Developing World: Supporting Education and Research
Presiding: Kym Faull, Giles Edwards
A408

This will be a follow-up to the workshops on the same topic presented at the 2017 and 2018 Indianapolis and San Diego ASMS meetings. The point will be to report on progress and interest during the preceding 12 months. Students in developing nations learn about mass spectrometry from text books. They rarely if ever get to actually see one, and never get to use them. Old but working instruments that are replaced with new versions could be made available to Universities and research organizations in developing countries to be used for research and teaching purposes. This would entail shipping, installation, training and maintenance which would all require funding and support. Some aspects of maintenance and training could probably be handled remotely via email, Skype, etc. This would be a noble aspiration for ASMS to embrace. It would improve our relations with the developing world and perhaps provide an example for other organizations (e.g. the NMR Society, etc) to follow. The Presiders will begin with a brief description of their personal experiences that stimulated them to organize this workshop. There is a need to formulate a plan of action that will assist with moving this initiative forward in the USA. There is a lot of interest but a way of cutting through the various layers of red tape that is currently impeding the mission is needed. All those interested are invited to join in a friendly and constructive discussion on this topic.

05 Ion Trap Mass Spectrometry: Latest Trends (Ion Trap MS Interest Group)
Presiding: Glen Jackson, Desmond Kaplan
A410

The Ion Trap Interest Group Meeting will cover the latest trends in instrumentation and applications in ion trap mass spectrometry. Instrumentation topics will cover some of the latest developments in instrument design, miniaturization, hybrid instruments and scanning methods. Applications will cover some of the latest trends in MSn, ion/molecule and ion/ion reaction methods. The workshop will consist of lightning-fast talks to introduce the topics and extended question and answer sessions to discuss, among other details, the limitations to commercialization of new advances.

06 FAIMS/DIMS/DMS Technology and its Impact on Current Day MS Analyses
Presiding: Sue Abbatiello
A307

The goal of this workshop is to provide a forum for people interested in High-field Asymmetric Waveform Ion Mobility Spectrometry (FAIMS) and Differential Ion Mobility Spectrometry (DIMS or DMS). We will go over the basics and fundamentals of how FAIMS/DIMS/DMS works, differences in hardware, the effects of different parameters on performance, and how it is different than Drift-Tube Ion Mobility (DT-IMS). Examples of applications benefiting from FAIMS/DIMS/DMS will be discussed, and attendees are invited to bring their questions and experiences of success, uncertainty, and even bad luck, to share with the community. Discussion will be led by several subject matter experts.

07 Food Safety and Quality Applications: Tools for Putting MS Methods into Practice
(Flavor Fragrance & Foodstuff Interest Group)
Presiding: Melanie Downs, James Redwine
A309

Mass spectrometry can be used to solve a number of different types of food safety and quality issues, but validation and implementation of methods across diverse food products and individual scenarios can be challenging. This workshop will discuss tools currently available and in development for food safety and quality MS analysis applications, including reference materials, method validation schemes, and other resources. The format of the workshop will include brief introductory presentations from selected resource developers and users, followed by a panel discussion moderated by the interest group co-chairs.

08 Automation for Proteomics Sample Preparation
Presiding: Michael Ford, Michael Knierman
A311

The performance of modern mass spectrometers and liquid chromatography systems is enabling proteomics experiments with previously unobtainable throughput and sensitivity. The analysis of cohorts of 50 or more samples, with acquisition timelines of a week or so, is now routine in many labs. Combined with robust sample preparation workflows and turnkey data processing proteomics is delivering on the promise and approaching a new level of usefulness. Assay and sample type aside it is fair to say, for proteomics experiments, the bottleneck is still instrument time. That said sample preparation is a significant use of human resources and with the scale of experiments expanding so too is the associated time and investment in labor. A practical solution to ease the growing sample preparation burden is automation.



5:45 - 7:00 PM MONDAY WORKSHOPS

There will be light refreshments in Building A foyers. All workshops are in Building A.

Automated sample preparation solutions are not new to the field of proteomics, look back ten years or so and 2D gel spot picking and in-gel digestion robots were common. Presently, and looking ahead, however the requirements of the field have changed; solution digestion, target enrichment at the protein and proteome level and sample clean-up are a few of the time-consuming tasks that would benefit from automation. Vendors have stepped up to deliver automation solutions such as the Agilent AssayMap, ThermoFisher KingFisher and more recent low cost OpenTrons OT2. This workshop is an opportunity to get together with like-minded scientists and discuss the emerging role of automation in sample preparation for proteomics experiments and to share practical experience with automation.

09 MS Software: Peak Picking - Paramount Practises and Perilous Pitfalls
Presiding: Magnus Palmblad, Jeff Agar
A312

The MS Software workshop is aimed at anyone who either writes MS software or is interested in learning how to. In this workshop, we will discuss the state of the art in peak picking, existing solutions, and common pitfalls.

Peak picking is a vital step in the interpretation of mass spectrometry data. Peak picking algorithms and their parameters influence your abundance accuracy, your false negative (missed peaks) and false positive (noise peaks erroneously detected that go on to be assigned) rates, and can even affect your mass accuracy. Peak shapes and the concept of spectral accuracy can be used to detect chimeric, unresolved, peaks and to help define instrument performance.

Peak picking, in the simplest sense, is the process of determining the mass-to-charge ratio (m/z) and abundance of peaks in mass spectra. When MS is hyphenated with other separation techniques, peak picking can be done on multidimensional data including tandem m/z, retention time or mobility. For the purposes of the discussion in this workshop, we will focus on the one-dimensional case of peaks in a mass spectrum.

When planning this year's workshop, we polled a number of stakeholders in the community. Peak picking was the most popular topic among those suggested. Learning from the feedback from the 2018 workshop, we will allocate most of the time to discussions and have only a short introduction to the topic. We will also discuss reference datasets with ground truth suitable for evaluating peak picking algorithms.

10 Solid Phase Microextraction Approaches Applied with Mass Spectrometry Techniques
Presiding: Janusz Pawliszyn
A313

The workshop is targeted at both new and current solid phase microextraction (SPME) users. The primary goal of this workshop is to provide interested participants with deeper insight into the main principles of this technique, which will ultimately enhance the productivity and quality of the analytical results. This workshop will be of interest to analytical and clinical chemists, laboratory supervisors, scientists and industry regulators in the environmental, food and beverage, pharmaceutical, clinical, forensic, cosmetic, and industrial hygiene fields. High throughput capabilities of the technology will be emphasized in the discussions including direct coupling to mass spectrometry via direct analysis in real time (DART), coated blade spray (CBS), microfluidic open interface (MOI) and others. The unique features of in vivo SPME sampling technologies will be of particular interest to researchers in biomedical, neurobiological and life sciences.

Agenda/Speakers

- Introduction to SPME and Bio-SPME; Janusz Pawliszyn (University of Waterloo)
- Ambient Ionization and SPME: A Perfect Complement; Robert B. (Chip) Cody (JEOL USA, Inc.)
- Rapid Determination of β-agonists in Animal Urine by Coated Blade Spray - Mass Spectrometry; Marco Blokland (RIKILT Wageningen University)
- Coated Blade Spray - Mass Spectrometry (CBS-MS) for Clinical Toxicology Testing in Urine; Shirin Hooshfar (University of California, San Francisco)
- *In vivo* SPME of Eicosanoids in Brain; Dajana Vuckovic (Concordia University)
- Determination of Cannabinoids using SPME Coupled to MS/LEI via MOI Interface; Achille Cappiello (University of Urbino)

12 LC-MS Jeopardy - I'll Take Increasing Throughput for $200 (LCMS & Related Topics Interest Group)
Presiding: Erik Soderblom, Will Thompson
A315

Need a break from formal talks? Already an expert in LC-MS and want to impress your friends? Not an expert and want to learn something about LC-MS? Just like games where you win "cash"? Well, this workshop is for you! Although the Jeopardy board has been cleared and refreshed from last year, the LC-MS and Related Topics Interest Group Workshop will remain focused on audience-driven discussions around various aspects of Proteomics, Pharmacokinetics, Metabolomics, Laboratory Automation, and Increasing Sample Throughput, all in a "Jeopardy" format! Early rounds will provide an opportunity to share, learn about, and discuss new and emerging strategies and applications in these various areas. Later rounds will be specific scenarios or analytical problems which are in need of solutions! Not only will creative, insightful, and thought provoking considerations be discussed, but will earn you and your team ASMS Jeopardy Cash (redeemable for free beers at ASMS Hospitality Suites).

13 Art and Cultural Heritage: Mass Spec Applications
Presiding: Mehdi Moini
A316

The purpose of this workshop is to discuss the application of MS to art and cultural heritage objects, as well as natural history specimens. This will be an interactive workshop in which various subjects relevant to museums' specimens will be discussed in a casual, dialog format. A preliminary list of topics include: 1) Analysis of paint, coating and binders; textiles; bone and tissue; ink and paper. 2) Mechanism of aging and degradation of art and natural history objects. 3) Dating. 4) Impact of radiation on museums' specimens. 5) Fossilomics and ancient DNA. 6) Forensic archeology. 7) Species identification of proteinaceous materials used in work of art and natural history. 8) Identification of forgery.

14 Photoionization (APPI/PI) - Bridging the Gap between Academic and Industrial Research (Photoionization MS Interest Group)
Presiding: Sven Ehlert, Eleanor Riches, Matthias Lorenz
A303

Photoionization is a powerful tool for soft ionization mass spectrometry (PI-MS) in research and routine analytical applications. After concentrating on the fundamentals of atmospheric pressure (APPI) and vacuum (SPI and REMPI) photoionization for mass spectrometry in the last year's workshop, we want to turn our view to the future of photoionization and discuss with the attendees challenges, ideas and new approaches. One or two key thought leaders will address the topic to stimulate discussion. The focus will be on the interface between academic and industrial research - what are the specific needs, capabilities and perspectives to bridge the gap with (AP)PI MS?
As a result of last year's workshop survey, we put the focus of this workshop on the discussion between participants. If it is appropriate and there is sufficient time, there will also be the chance for attendees to share novel and exciting developments with the PI community. Furthermore, we want to give attendees with different experience levels the opportunity to get in contact to discuss challenges as well as ask questions to the experts and more experienced users.

There will be light refreshments in Building A foyers. All workshops are in Building A.

Together with the attendees, we want to reveal the advantages, capabilities and diversity of photoionization mass spectrometry to support its dissemination into laboratories worldwide.

15 MS-Based Multi-Attribute Method (MAM): The Future of Biotherapeutic Development Analytics
(Biotherapeutics Interest Group)
Presiding: Andrew Dawdy, Hao Zhang
A302

Join our panel of experts to discuss the future of MAM, an emerging mass spectrometry-based methodology with the potential to significantly transform standard analytical practice for biotherapeutic development across the biopharma industry. In the development of biotherapeutics, a thorough understanding of a molecule's product quality attributes (PQAs) and their effect on its structure and function is essential for ensuring safety and efficacy of the clinical trial material. Numerous routine chromatographic and electrophoretic assays, intended for batch release, are used to characterize and monitor the PQAs that contribute to product-related heterogeneity such as N-glycosylation, charge isoforms, oxidation, fragmentation, and aggregation. However, execution of multiple routine methods for batch release, stability time-points, and process/formulation development support becomes time and resource intensive, and often provides an indirect measure of biologically-relevant PQAs. Recently, a liquid chromatography-mass spectrometry-based multi-attribute method (MAM) has arisen (Rogers et al., AAPS J, 2017) as an improved means for detecting, identifying, and quantitating a multitude of PQAs in an automated fashion by a single assay. In its short public lifespan, MAM's popularity has exploded as evidenced by the formation of an industry-wide MAM Consortium, assessment of its suitability by the FDA, and the rapid growth in MAM-centric products from numerous vendors. MAM is poised to revolutionize the biopharmaceutical industry if fully embraced and adopted. This workshop will provide a forum to discuss the status of MAM and address existing challenges. Topics may include sample preparation, instrumentation, software/data processing, hotspot characterization, new peak detection, regulatory acceptance, qualification and validation, and more.

16 MS Career Options: How to Kick Start Your Career
(Young Mass Spectrometrists Interest Group)
Presiding: Veronica Anania, Sharon Pitteri
A301

This workshop features a panel discussion on professional development in the area of mass spectrometry. Topics will be focused on career planning and management, fundamental training, industrial internship, job search tools and interview strategies. The panel, consisting of representatives from industrial and academic organizations, will share their knowledge and practices on career prospects.

17 Membrane Proteins, Nanodiscs, and Beyond: MS Analysis in Academia and Industry
Presiding: Iain Campuzano, Michael Marty
A305

Membrane proteins make up over 50% of possible "druggable" targets, making them very attractive targets for academic and industrial research. Membrane proteins are inherently insoluble in aqueous solvents and require the presence of lipid or detergent to remain soluble, which makes their analysis by many biophysical techniques such as native mass spectrometry (MS) and x-ray crystallography very challenging. However, over the past 10 to 15 years, researches have begun to overcome such hurdles and are now producing native intact mass spectra for membrane protein complexes of ion channels, membrane bounds receptor molecules, transporters, and fully assembled lipoprotein nanodiscs.
Most of this pioneering work has been focused on native MS in the academic environment. Native MS analysis of membrane proteins within the pharmaceutical industry is still in its infancy compared to established structural biology techniques such as x-ray diffraction and cryo-EM.

Within this workshop, we will discuss MS experiments for characterizing intact membrane proteins under denaturing and native conditions, focusing on current protocols used within both academia and industry for native MS analysis of membrane protein solubilized in "MS-friendly" detergents. We will also discuss how these techniques can be used to support the structural biology and drug discovery efforts within the pharmaceutical industry.

The workshop will be a panel discussion format where general and detailed topics can be discussed.
A preliminary list of discussion topics will include:

- MS determination of membrane proteins using denaturing LC and MS conditions
- Membrane protein purification and detergent screening for optimal MS analysis
- Native MS instrumentation and analysis of membrane proteins
- New frontiers in membrane mimetics: nanodiscs and beyond
- The industrial perspective on membrane protein MS

18 Energy, Petroleum, and Biofuels MS: Targeted Analysis, Fingerprinting and Speciation in Complex Mixtures
(Energy Petroleum & Biofuels Interest Group)
Presiding: Marianny Combariza, Amy McKenna
A304

Fossil- and bio- fuels are complex mixtures containing thousands of compounds with different molecular compositions; which in turn determine macroscopic properties. In petroleum chemistry, for instance, low MW components of low and medium polarity are well studied and understood. However, trace amounts of heavier and polar components, less known compositionally, are usually very reactive and responsible for many problems. For instance, asphaltenes, naphthenic acids and metal complexes can cause aggregate formation, corrosion and catalyst poisoning, during transport, storage and refining of petroleum. Yet, due to lower ionization efficiencies than their low MW counterparts, these compounds remain undetected in direct infusion MS analysis of the whole oil.

Correlating compositional data to macroscopic behavior is paramount to future energy research, with HRMS playing a vital role at providing molecular information. Complex organic mixture analysis by MS has prompted development of novel ionization sources and techniques, off- and on-line chromatographic methods, and data processing algorithms. Despite many efforts to overcome the limitation of ion suppression in these polydisperse systems, compound classes present in low concentration still remain undetected. Often, these species are responsible for performance issues of final products derived from the raw feeds. Therefore, targeted analysis, fingerprinting and selective speciation of chemical functional groups is emerging as the next big advancement in MS of complex mixtures. In this workshop, practitioners from these areas will present the development and applicability of their strategies of analysis, and will participate in a panel discussion with the audience.

Topics: Selective ionization, selective fractionation, derivatization, structure-related separation.

From 7:00 am Tuesday
CORPORATE BREAKFAST SEMINARS
CONVENTION CENTER AND OMNI CNN CENTER HOTEL
See page 16 for detailed schedule. Reservation or RSVP required.

8:30 - 10:30 pm Tuesday
INFORMATICS: INNOVATIONS
Session Chair: David Stranz (Sierra Analytics, Inc.)
Murphy Ballroom, Bldg B, Level 5

TOA am 08:30 **Differential Mass Spectra (ΔS) and Differential Ion Currents (ΔIC) for Smarter Mass Spectrometer Operation and Data Interpretation;** Changtong Hao[1]; Thomas Lee Collier[1,2]; Lawrence Klecha[1]; Simon Prosser[1]; Daniel Eikel[1]; *[1]Advion Inc., Ithaca, NY; [2]Harvard Medical School, Boston, MA*

TOA am 08:50 **XNet: A Bayesian Approach to Extracted Ion Chromatogram Clustering for Precursor Mass Spectrometry Data;** Mathew M Gutierrez[1]; Kyle Handy[1]; Rob Smith[1]; *[1]University of Montana Missoula, MT*

TOA am 09:10 **KairosMS: Processing of Complex Mixture Data Analyzed by Hyphenated Ultrahigh Resolution Mass Spectrometry;** Remy Gavard[1]; Hugh E. Jones[1]; Diana Catalina Palacio Lozano[1]; Mary J. Thomas[1]; David Rossell[1,2]; Simon E. F. Spencer[1]; Mark P. Barrow[1]; *[1]University of Warwick, Coventry, United Kingdom; [2]Universitat Pompeu Fabra, Barcelona, Spain*

TOA am 09:30 **Zero-Knowledge *de novo* and the Alphabet Projection of Spectra;** Patrick Kreitzberg[1]; Marshall Bern[2]; Oliver Serang[1]; *[1]University of Montana, Missoula, MT; [2]Protein Metrics Inc., San Carlos, CA*

TOA am 09:50 **Fast and Accurate Estimation of Relative Molecule Abundance and Resolution of Overlapping Isotopic Envelopes Using Optimal Transport Theory;** Michał Aleksander Ciach[1,2]; Grzegorz Skoraczyński[1]; Szymon Majewski[3]; Błażej Miasojedow[1]; Michał Piotr Startek[1]; Dirk Valkenborg[2,4,5]; Anna Gambin[1]; *[1]Faculty of Mathematics, Informatics and Mechanics, University of Warsaw, Warsaw, Poland; [2]Centre for Statistics, Hasselt University, Diepenbeek, Belgium; [3]Mathematical Institute of the Polish Academy of Sciences, Warsaw, Poland; [4]UA-VITO Center for Proteomics, University of Antwerp, Antwerp, Belgium; [5]Applied Bio and Molecular Systems, Flemish Institute for Technological Research (VITO), Mol, Belgium*

TOA am 10:10 ***ab initio* Prediction of Peptide Tandem Mass Spectra;** Kaiyuan Liu[1]; Sujun Li[1]; Lei Wang[1]; Yuzhen Ye[1]; Haixu Tang[1]; *[1]Indiana University, Bloomington, IN*

8:30 - 10:30 pm Tuesday
FUNDAMENTALS: PHOTOIONIZATION AND PHOTODISSOCIATION
Session Chair: Hendrik Kersten (University of Wuppertal)
B401-402

TOB am 08:30 **APPI-MS Analysis of Endohedral Fullerenes;** Julie Herniman[1]; G. John Langley[1]; Sally Bloodworth[1]; Richard J Whitby[1]; Gabriela Sitinova[1]; *[1]University of Southampton, Southampton, United Kingdom*

TOB am 08:50 **Right-Angle Ion Mirror-Prism (RAIMP): First Experiments with the Novel Time-of-Flight Mass Analyzer;** Igor V. Veryovkin[1]; Raveendra C. Wickramasinghe[1]; Igor L. Bolotin[1]; Jason M. Gross[1]; C. Emil Tripa[1]; Luke Hanley[1]; *[1]University of Illinois at Chicago (UIC), Chicago, IL*

TOB am 09:10 **Improved Top-Down *de novo* Sequencing of Denatured and Native Proteins Using Hybrid Ion Activation Methods;** Weijing Liu[1]; Kira Vyatkina[2]; Jared B. Shaw[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]St. Petersburg Academic University, St. Petersburg, Russia*

TOB am 09:30 **Peptide and protein fragmentation using 193 nm UVPD on a Q-IM-TOF platform;** Alyssa Q. Stiving[1,2]; Sophie R. Harvey[1,2]; Benjamin J. Jones[2,3]; Bruno Bellina[4]; Perdita E. Barran[5]; Jeffery M. Brown[6]; Vicki H. Wysocki[2,3]; *[1]The Ohio State University, Columbus, OH; [2]Resource for Native Mass Spectrometry Guided Structural Biology, The Ohio State University, Columbus, OH; [3]The Ohio State University, Columbus, OH; [4]Manchester Institute of Biotechnology, University of Manchester, United Kingdom; [5]Manchester Institute of Biotechnology, University of Manchester, United Kingdom; [6]Waters Corporation, Wilmslow, United Kingdom*

TOB am 09:50 **Enhanced Characterization of Membrane Protein Complexes Using Ultraviolet Photodissociation;** Sarah N Sipe[1]; John W Patrick[2]; Arthur Laganowsky[2]; Jennifer S Brodbelt[1]; *[1]Department of Chemistry, University of Texas, Austin, TX; [2]Department of Chemistry, Texas A&M University, College Station, TX*

TOB am 10:10 **Chiral Analysis Base on Mass Spectrometry and Photodissociation Spectroscopy in the Gas Phase: from IR to UV;** Xianglei Kong; *Nankai University, Tianjin, China*

8:30 - 10:30 pm Tuesday
NATIVE MS IN STRUCTURAL BIOLOGY
Session Chair: Rita Grandori (University of Milano-Bicocca)
B405-407

TOC am 08:30 **Native MS-Based Platform for Screening Optimal Conditions in Preparing Intact Macromolecular Assemblies for cryo-EM Analysis;** Paul Dominic B. Olinares[1]; Courtney Chiu[2]; Jin Young Kang[2]; Eliza Llewellyn[2]; James Chen[2]; Ruth Saecker[2]; Elizabeth Campbell[2]; Seth Darst[2]; Brian T. Chait[1]; *[1]Laboratory of Mass Spectrometry & Gaseous Ion Chemistry, The Rockefeller University, New York, NY; [2]Laboratory of Molecular Biophysics, The Rockefeller University, New York, NY*

TOC am 08:50 **Exploring the Structure and Specificity of Antimicrobial Peptides in Lipid Nanodiscs by Native MS;** Larry Walker[1]; Elaine Marzluff[2]; Marius Kostelic[1]; Julia Townsend[1]; Michael Thomas Marty[1]; *[1]University of Arizona, Tucson, AZ; [2]Grinnell College, Grinnell, IA*

TOC am 09:10 **Interaction of Metals with Amyloid Beta and Alpha-Synuclein Studied by Native FTICR-MS with Advanced Dissociation Methods;** Frederik Lermyte[1]; Francesca Bellingeri[1]; James Everett[2]; Jake Brooks[1]; Yuko P. Y. Lam[1]; Christopher A. Wootton[1]; Mark P. Barrow[1]; Peter J. Sadler[1]; Neil D. Telling[2]; Joanna F. Collingwood[1]; Peter B. O'Connor[1]; *[1]University of Warwick, Coventry, United Kingdom; [2]Keele University, Stoke-on-Trent, United Kingdom*

TOC am 09:30 **Development of High Throughput Online Native LC/MS;** Chris Nortcliffe[1]; Esme Candish[2]; Sibylle Heidelberger[3]; Ferran Sanchez[4]; Sean McCarthy[2]; *[1]AB Sciex UK Ltd, Warrington, United Kingdom; [2]Sciex, Framingham, MA; [3]SCIEX, Warrington, United Kingdom; [4]SCIEX, Darmstadt, Germany*

TOC am 09:50 **Analysis of Diubiquitin Chains by Variable-Temperature Electrospray Ionization Provides Evidence for Seven Non-Native Solution States and Stabilities;** Lucas W. Henderson[1]; Tarick J. El-Baba[1]; Shannon A. Raab[1]; Christopher J. Brown[1]; Daniel W. Woodall[1]; David E. Clemmer[1]; *[1]Department of Chemistry, Indiana University, Bloomington, IN*

TOC am 10:10 **Multistage Native MS Enables Direct Identification of Unknown Ligands Bound to Protein Assemblies;** Joseph F Gault[1]; Idlir Liko[2]; Michael Landreh[3]; Hsin-Yung Yen[2]; Denis Shutin[1]; Rosa Viner[4]; Romain Huguet[4]; Christopher Mullen[4]; John E. P. Syka[4]; Jesse D Canterbury[4]; Philip M Remes[4]; Graeme McAlister[4]; Carol V. Robinson[1]; *[1]Oxford University, Oxford, United Kingdom; [2]OMass Therapeutics, Oxford, United Kingdom; [3]Karolinska Institutet, Stockholm, Sweden; [4]Thermo Fisher Scientific, San Jose, CA*

8:30 - 10:30 pm Tuesday
IMAGING: PHARMACEUTICALS, METABOLITES, AND LIPIDS
Session Chair: Uwe Karst (University of Münster)
B302-305

TOD am 08:30 **High-Performance MS Strategies Provide Detailed Insights into Neglected Tropical Diseases and Infection Mechanisms;** Bernhard Spengler[1]; Stefanie Gerbig[1]; Patrik Kadesch[1]; Parviz Ghezellou[1]; Simone Häberlein[2]; Christoph G. Grevelding[2]; Katja Becker[3]; Anja Taubert[2]; Carlos Hermosilla[2]; *[1]Analytical Chemistry, Giessen, Germany; [2]Institute of Parasitology, Giessen, Germany; [3]Biochemistry and Molecular Biology, Giessen, Germany*

TOD am 08:50 **MALDI Mass Spectrometry Imaging of Alzheimer's Disease Human Brain Tissue Reveals Distributions of Functionally Important Metabolites;** Abby S. Gelb[1, 2]; Nivedita Bhattacharya[2]; Weiming Xia[1, 2]; Catherine E. Costello[2]; *[1]Edith Nourse Rogers Memorial Veterans Hospital, Geriatric Research Education & Clinical Center, Bedford, MA; [2]Boston University School of Medicine, Boston, MA*

TOD am 09:10 **Lessons Learned from Mice and Cheese: Investigating Diffusion Processes by MALDI MS Imaging;** Julia Kokesch-Himmelreich[1]; Alan M. Race[1]; Axel Treu[1]; Claus Schlicht[2]; Ulrich Busch[2]; Kerstin Walter[3]; Christoph Hölscher[3]; Andreas Römpp[1]; *[1]University of Bayreuth, Bayreuth, Germany; [2]Bavarian Health and Food Safety Authority, Oberschleißheim, Germany; [3]Research Center Borstel, Borstel, Germany*

TOD am 09:30 **Simultaneous Lipids/Metabolites Imaging (1 µm Resolution) of Traumatic Brain Injury Tissue Using Gas Cluster Ion Beam Secondary Ion Mass Spectrometry (GCIB-SIMS);** Hua Tian[1]; Louis J. Sparvero[2, 3]; Andrew A. Amoscato[2, 4]; Valerian E. Kagan[2, 4, 5]; Hülya Bayır[2, 4, 6]; John C. Vickerman[7]; Peter J. Cumpson[8]; Nicholas Winograd[1]; *[1]Department of Chemistry, Pennsylvania State University, University Park, PA; [2]Department of Environmental and Occupational Health, University of Pittsburgh, Pittsburgh, PA; [3]Center for Free Radical and Antioxidant Health, Pittsburgh, PA; [4]Center for Free Radical and Antioxidant Health, University of Pittsburgh, Pittsburgh, PA; [5]Departments of Chemistry, Pharmacology and Chemical Biology, Radiation Oncology, University of Pittsburgh, Pittsburgh, PA; [6]Department of Critical Care Medicine, and Safar Center for Resuscitation Research, University of Pittsburgh, Pittsburgh, PA; [7]School of Chemical Engineering and Analytical Science, The University of Manchester, Manchester, United Kingdom; [8]Mark Wainwright Analytical Centre, he University of New South Wales, Sydney, Australia*

TOD am 09:50 **Dual Mode Mass Spectrometry Imaging to Probe the Inflammatory Properties of Nanoparticle Stabilized Capsules;** Kristen Sikora[1]; Joseph M Hardie[1]; Vincent M Rotello[1]; Richard W. Vachet[1]; *[1]University of Massachusetts, Amherst, MA*

TOD am 10:10 **Correlated Chemical Mapping of Multiple Compounds and Metabolites in Rat Tissues;** Gary J Van Berkel[1]; Thomas R. Covey[2]; Chang Liu[2]; Bryce Young[2]; Robert Johnson[3]; Christopher DeBenedetto[3]; Danielle Diaz[3]; Adam Bentley[3]; James Glick[3]; Jimmy Flarakos[3]; *[1]Gary Van Berkel LLC, Oak Ridge, Tennessee; [2]SCIEX, Concord, ON; [3]Novartis Institutes for BioMedical Research, East Hanover, NJ*

8:30 - 10:30 pm Tuesday
ENVIRONMENTAL: EMERGING CONTAMINANTS
(IN HONOR OF RON HITES)
Session Chair: Susana Y. Kimura (University of Calgary)
B308-309

TOE am 08:30 **Nontargeted Identification of Antioxidants in the Environment;** Ronald A. Hites[1]; Yan Wu[1]; Marta Venier[1]; *[1]Indiana University, Bloomington, IN*

TOE am 08:50 **Stable Isotopic Labeling and Nontargeted Identification of ng/L Amino-Contaminants in Water;** Zhongshan Liu[1]; Guang Huang[1]; Ping Jiang[1]; Lindsay Jmaiff Blackstock[1]; Xing-Fang Li[1]; *[1]University of Alberta, Edmonton, AB*

TOE am 09:10 **Organic Pollutants in the Snow of Franz Joseph Land. Expedition 2017;** Dmitrii Mazur[1, 2]; Dmitrii Kosyakov[2]; Aleksandr Kozhevnikov[2]; Thomas Latkin[2]; Evgeniy Varakin[2]; Oleg Khoroshev[2]; Albert T Lebedev[1]; *[1]Moscow State University, Moscow, Russia; [2]Lomonosov Northern (Arctic) Federal University, Centre of collective usage "Arctica", Arkhangelsk, Russia*

TOE am 09:30 **Design and Initial Findings of EPA's Non-Targeted Analysis Collaborative Trial (ENTACT);** Jon R Sobus[1]; Elin Ulrich[2]; Jarod Grossman[3, 4]; Alex Chao[3]; Randolph Singh[5, 6]; Christopher Grulke[7]; Ann Richard[7]; Andrew McEachran[5]; Seth Newton[2]; Mark Strynar[2]; Kamel Mansouri[5, 6]; Antony Williams[7]; *[1]US EPA, Research Triangle Park, NC; [2]US EPA, National Exposure Research Laboratory, Research Triangle Park, NC; [3]Student Contractor, US EPA, Research Triangle Park, NC; [4]Agilent Technologies, Inc., Santa Clara, CA; [5]ORISE Participant, US EPA, Research Triangle Park, NC; [6]University of Luxembourg · Luxembourg Centre for Systems Biomedicine (LCSB), Luxembourg City, Luxembourg; [7]US EPA, National Center for Computational Toxicology, Research Triangle Park, NC; [8]Integrated Laboratory Systems, Inc., Contractor to National Toxicology Program, National Institute of Environmental Health Sciences, Morrisville, NC*

TOE am 09:50 **Multidimensional Fractionation and Molecular Characterization of Lingering Oil Compounds in Coastal Sediments: A Nine Year Evolution;** Amy McKenna[1]; Huan Chen[1]; Cameron C. Davis[1]; Donald F Smith[1]; Sydney Niles[1, 2]; Chad R. Weisbrod[1]; Gregory T. Blakney[1]; Aixin Hou[3]; Qianxin Lin[3]; Ryan P. Rodgers[1, 2]; *[1]National High Magnetic Field*

Laboratory, Florida State University, Tallahassee, FL; [2]Florida State University, Tallahassee, FL; [3]Louisiana State University, Baton Rouge, LA

TOE am 10:10 **Advancing a Full Picture on Water-Soluble Synthetic Polymers in Wastewater- Different Ionization Strategies for Homologue Series Detection**; Teresa Mairinger[1]; Martin Loos[2]; Juliane Hollender[1, 3]; *[1]EAWAG: Swiss Federal Institute of Aquatic Science and Technology, Dübendorf, Switzerland; [2]looscomputing, Zurich, Switzerland; [3]Institute of Biogeochemistry and Pollutant Dynamics, ETH Zurich, Zurich, Switzerland*

8:30 - 10:30 pm Tuesday
PROTEIN-LIGAND INTERACTIONS
Session Chair: Justin Benesch (University of Oxford)
B312-314

TOF am 08:30 **Semi-Tryptic Peptide Enrichment Strategy for Protein-Ligand Interaction Analysis on the Proteomic Scale Using Limited Proteolysis**; Michael C. Fitzgerald[1]; Renza Ma[1]; Do-Yeon Kwon[1]; Tesia Stevenson[1]; Hyeri Park[1]; Jiyong Hong[1]; *[1]Duke University, Durham, NC*

TOF am 08:50 **Interactions between Integrin and Ligands: Conformational Changes upon Binding to RDG-type receptors**; Roxana E. Iacob[1]; Yang Su[2]; Timothy A. Springer[3]; John R. Engen[1]; *[1]Northeastern University, Boston, MA; [2]Harvard Medical School, Boston, MA; [3]Harvard Medical School, Boston, MA*

TOF am 09:10 **A Single Experiment (LITPOMS) Reveals Composite Conformational Changes, Order of Binding, and Affinities for Calcium Binding to Calmodulin**; Roger (Xiaoran) Liu[1]; Mengru Zhang[1]; Don L. Rempel[1]; Michael L. Gross[1]; *[1]Washington University, St. Louis, MO*

TOF am 09:30 **Ion Mobility-Mass Spectrometry of Peptidomimetic-Aβ Complexes: Towards Generalized Amyloid Inhibitors**; Yilin Han[1]; Neha Jain[2]; Varun V. Gadkari[3]; Elizabeth Gichana[3]; Fredrick Almqvist[4]; Magdalena I. Ivanova[3]; Matthew T. Chapman[3]; Brandon T. Ruotolo[3]; *[1]Univeristy of Michigan, Ann Arbor, MI; [2]Ahmedabad University, Ahmedabad, India; [3]University of Michigan, Ann Arbor, MI; [4]Umeå University, Umeå, Sweden*

TOF am 09:50 **Combining Native Mass Spectrometry with Ion Mobility and Top-Down Approaches Provides Unique Insights into the Dynamics of Protein-RNA Interactions**; Rebecca J. D'Esposito[1]; Alice Sosic[1]; Daniele Fabris[1]; *[1]The RNA Institute, University at Albany, Albany, NY*

TOF am 10:10 **Quantifying Soluble Protein Interactions with Glycolipids in Model Membranes**; Ling Han[1]; Michele Richards[1]; Elena N Kitova[1]; John Klassen[1]; *[1]University of Alberta, Edmonton, AB*

8:30 - 10:30 pm Tuesday
MS IN THE QC LAB
Session Chair: Richard Rogers (Just Biotherapeutics)
Auditorium, Bldg A

TOG am 08:30 **A Software Tool for Automated, Fast, Flexible and Comprehensive Quality Control Analysis of Shotgun Proteomics Raw-Files**; Christian D. Kelstrup[1]; Martin Rykaer[1]; Jeppe Madsen[1]; Jesper V. Olsen[1]; *[1]CPR, University of Copenhagen, Copenhagen N, Denmark*

TOG am 08:50 **QC Benchmarker: A Streamlined Web Application to Comprehensively Evaluate Instrument Performance and Direct Troubleshooting**; Benjamin Neely[1]; Magnus Palmblad[2]; *[1]National Institute of Standards and Technology, Charleston, SC; [2]Leiden University Medical Center, Center for Proteomics and Metabolomics, Leiden, Netherlands*

TOG am 09:10 **Multi-Attribute Method Evaluation of the High Resolution X500B Quadrupole Time-of-Flight System**; Monica Sadek[1]; Frank Macchi[1]; Chengfeng Ren[1]; Benjamin Moore[1]; *[1]Genentech, Inc., South San Francisco, CA*

TOG am 09:30 **Meeting the Challenges of Implementing Accurate-Mass Mass Spectrometry for Biotherapeutic Development in Regulated/ Non-Regulated Environments**; Henry Shion[1]; Mellisa Ly[2]; Nilini Ranbaduge[1]; Ximo Zhang[1]; Yun Adelyunas[1]; Jonathan Pugh[3]; Robert Lewis[3]; Jill Lord[3]; Mark Halifax[3]; Nick Tomczyk[3]; Ying-Qing Yu[1]; Jason Rouse[2]; Weibin Chen[1]; *[1]Waters Corporation, Milford, MA; [2]Pfizer, Andover, MA; [3]Waters Corporation, Wilmslow, United Kingdom*

TOG am 09:50 **Understanding Biotherapeutic Product Quality Attributes through a Multi-Attribute Method (MAM) Lab-of-the-Future**; Andrew William Dawdy[1]; Kristin Boggio[2]; Keith Lutke[1]; Anastasiya Manuilov[2]; Tiffany Medwid[1]; Halyna Narepekha[1]; Wenqin Ni[2]; Nataliya Parahuz[1]; Himakshi Patel[2]; Thomas Powers[1]; David Ripley[2]; Amy Schmidt[2]; Justin Sperry[1]; Matthew Thompson[2]; Joshua Woods[1]; Ying Zhang[2]; Richard Cornell[2]; Sonia Taktak[2]; Carly Daniels[1]; Keith Johnson[2]; Olga Friese[1]; Jason Rouse[2]; *[1]Pfizer, Chesterfield, MO; [2]Pfizer, Andover, MA*

TOG am 10:10 **Strategies and Practices for Implementing Multi-Attribute Method (MAM) in GMP Environment**; Da Ren; *Amgen Inc., Thousand Oaks, CA*

8:30 - 10:30 pm Tuesday
NUCLEIC ACIDS AND OLIGONUCLEOTIDES
Session Chair: Satoko Akashi (Yokohama City University)
A411-412

TOH am 08:30 **Nucleic Acids Biophysics by In-Solution HDX/ Native MS**; Eric Largy[1]; Laura Fricot[1]; Anaïs Ferrer[1]; Valérie Gabelica[1]; *[1]Université de Bordeaux, INSERM U1212, CNRS UMR 5320, IECB, Pessac, France*

TOH am 08:50 **Duplex and Triplex siRNA-mAb Conjugate Product Confirmation for Pharma: Positive or Negative Native nESI MS**; Iain D G Campuzano[1]; Carter Lantz[2]; Chawita Netirojjanakul[3]; Sara C Humphreys[4]; Mai B Thayer[4]; Joseph A Loo[2]; *[1]Amgen Inc., Thousand Oaks, CA; [2]UCLA, Los Angeles, CA; [3]Amgen, Inc., Thousand Oaks, CA; [4]Amgen, South San Francisco*

TOH am 09:10 **Combining Different Solution Denaturation Techniques to Expand the Limits of Top-Down Analysis of Large Ribonucleic Acids**; Will McIntyre[1]; Thomas Kenderdine[1]; Botros Toro[1]; Ryan Treen[1]; Alice Sosic[1]; Daniele Fabris[1]; *[1]SUNY Albany, NY*

TOH am 09:30 **Using Nucleic Acid Stable Isotope Labeling Mass Spectrometry (NAIL-MS) to Unlock the Mysteries Surrounding RNA Modifications**; Kayla Borland[1]; Felix Hagelskamp[1]; Valentin Reichle[1]; Matthias Heiss[1]; Stefanie Kellner[1]; *[1]Ludwig-Maximilians-University, Munich, Germany*

TOH am 09:50 **The Landscape of Post-Transcriptional Modifications in Human tRNA**; Hendrik Weisser[1]; Jack Rogan[1]; Byron Andrews[1]; *[1]STORM Therapeutics Limited, Cambridge, United Kingdom*

TOH am 10:10 **The Role of Bioanalytical Assays in Supporting the Development of a siRNA Nanoparticle Drug;** Uma Kavita[1]; Neil Mathias[1]; Fulya Akpinar[1]; Giridhar S. Tirucherai[1]; Renuka C. Pillutla[1]; Qin C. Ji[1]; *[1]Bristol-Myers Squibb Co., Princeton, NJ*

10:30 am - 2:30 pm Tuesday

TUESDAY POSTER SESSION
Poster/Exhibit Hall ground level
Lunch concessions are open 11:00 am - 2:00 pm

Odd-number posters present:
10:30 am - 11:30 am PLUS 12:30 - 2:30 pm

Even-number posters present:
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Poster Pick-Me-Up Snacks served at 1:30 pm



TUESDAY AFTERNOON ORAL SESSIONS

2:30 - 4:30 pm Tuesday
INFORMATICS: DATA-INDEPENDENT ACQUISITION
Session Chair: Bernd Wollscheid (Institute of Molecular Systems Biology, ETH Zürich)
Murphy Ballroom, Bldg B, Level 5

TOA pm 02:30 **Mobi-DIK (Ion Mobility DIA Analysis Kit): Targeted Analysis Software for diaPASEF Data Improves Proteome Coverage;** Annie Ha[1]; Max Frank[1]; Florian Meier[2]; Andreas-David Brunner[2]; Stephanie Kaspar-Schönefeld[3]; Scarlet Koch[3]; Markus Lubeck[3]; Oliver Raether[3]; Ben C Collins[4]; Ruedi Aebersold[4]; Matthias Mann[2, 5]; Hannes Röst[1]; *[1]Donnelly Centre for Cell and Molecular Research, University of Toronto, Toronto, ON; [2]Max Planck Institute of Biochemistry, Martinsried, Germany; [3]Bruker Daltonik GmbH, Bremen, Germany; [4]ETH Zurich, Zurich, Switzerland; [5]NNF Center for Protein Research University of Copenhagen, Copenhagen, Denmark*

TOA pm 02:50 **"Library-Free" DIA Analysis: Using Proteome-Wide in-silico Generated Spectral Libraries by Prosit for DIA Data Analysis;** Tobias Schmidt[1]; Daniel P Zolg[1]; Siegfried Gessulat[1, 2]; Oliver M. Bernhardt[3]; Tejas Gandhi[3]; Patroklos Samaras[1]; Martin Frejno[1]; Hans-Christian Ehrlich[2]; Lukas Reiter[3]; Bernhard Kuster[1]; Mathias Wilhelm[1]; *[1]Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; [2]SAP SE, Potsdam, Germany; [3]Biognosys, Schlieren, Switzerland*

TOA pm 03:10 **Increasing the Dynamic Range of Data Independent Acquisition (DIA) by Fusing BoxCar MS1 With Segmented MS2;** Florian Meier[1]; Roland Bruderer[2]; Oliver M. Bernhardt[2]; Tabiwang N. Arrey[3]; Tejas Gandhi[2]; Yue Xuan[4]; Oliver Lange[3]; Alexander Makarov[3]; Alexander Harder[3]; Lukas Reiter[2]; Matthias Mann[1]; *[1]Max Planck Institute of Biochemistry, Martinsried, Germany; [2]Biognosys AG, Schlieren, Switzerland; [3]Thermo Fisher Scientific, Bremen, Germany; [4]Thermo Fisher Scientific, Bremen, Germany*

TOA pm 03:30 **Avant-Garde: Your DIA Data Sommelier to Assess and Improve Quantitative Suitability in Large Datasets;** Sebastian Vaca[1]; Karen E. Christianson[1]; Nicholas Schulman[2]; Karsten Krug[1]; Katherine C. DeRuff[1]; Ryan Peckner[1]; Malvina Papanastasiou[1]; Michael J. MacCoss[2]; Jacob D. Jaffe[1]; Steven A. Carr[1]; *[1]Broad Institute of MIT and Harvard, Cambridge; [2]University of Washington, Seattle, WA*

TOA pm 03:50 **ISObaric Modification Extraction and Resolvement (ISOMER);** Zuofei Yuan[1]; Simone Sidoli[1]; Katarzyna Kulej[1, 2]; Benjamin A. Garcia[1]; *[1]University of Pennsylvania, Philadelphia, PA; [2]The Children's Hospital of Philadelphia, Philadelphia, PA*

TOA pm 04:10 **An Open Searching Strategy for Identification and Quantification of Expressed Variants in Serum and Plasma;** Matthew Foster[1]; Emily Ko[1]; J. Will Thompson[1]; Sunil Suchindran[1]; Sarah Rains[1]; Rose Asrican[1]; L. Gayani Tillekeratne[1]; Matthew Rubach[1]; Thomas Burke[1]; Elizabeth Petzold[1]; Christopher Woods[1]; M. Arthur Moseley[1]; *[1]Duke University, Durham, NC*

2:30 - 4:30 pm Tuesday
GC/MS, GCXGC/MS, GC-MS/MS, AND GC/HRMS
Session Chair: David Touboul (CNRS-ICSN)
B401-402

TOB pm 02:30 **Enantiomeric Profiling of Terpenes in Plant Material Using Gas Chromatography-Mass Spectrometry;** Seamus Riordan-short[1]; Don Nguyen[1]; Thu-Thuy Dang[1]; Rob O'Brien[1]; Matthew Noestheden[1]; *[1]Supra R&D, Kelowna, BC*

TOB pm 02:50 **Evaluating the Volatile Constituents of Different Cannabis Varieties using Solventless Sample Preparation and Orbitrap Based MS Detection;** Gyorgy Vas; *VasAnalytical, Flemington, NJ*

TOB pm 03:10 **Covalent Adduct Chemical Ionization (CACI-) MS/MS for Assignment of Double Bond Position without Standards on a Shimadzu Triple Quadrupole MS;** Tom Brenna[1]; Hui Gyu Park[1]; Zhen Wang[1]; Dong Hao Wang[1]; Riki Kitano[2]; *[1]University of Texas, Austin, TX; [3]Shimadzu Scientific Instruments, Inc., Columbia, MD*

TOB pm 03:30 **Extending the Range of Compounds Amenable for GC-MS Analysis with Cold EI – Recent Applications;** Aviv Amirav[1]; Alexander B. Fialkov[1]; Ksenia Kladchenko[1]; Tal Alon[1]; *[1]Tel-Aviv University, Tel-Aviv, Israel*

TOB pm 03:50 **Large Scale Breath Monitoring for Asthma Phenotyping;** Jean-François Focant[1]; Delphine Zanella[1]; Pierre-Hugues Stefanuto[1]; Florence Schleich[2]; Renaud Louis[2]; *[1]Liège University, Liege, Belgium; [2]Liège University Hospital, Liège, Belgium*

TOB pm 04:10 **GNPS GC Enables Automated Processing, Annotation and Visualization of Large Scale GC-MS Metabolomics Datasets**; Alexander Aksenov[1]; Ivan Laponogov[2]; Mingxun Wang[3]; Dennis Veselkov[4]; Zheng Zhang[3]; Louis Felix Nothias[3]; Alexey Melnik[3]; Pieter Dorrestein[3]; Kirill Veselkov[2]; *[1]UCSD, La Jolla, CA; [2]Imperial College London, London, United Kingdom; [3]University of California San Diego, La Jolla, CA; [4]Intelligify Limited, London, United Kingdom*

2:30 - 4:30 pm Tuesday
TOP DOWN PROTEIN ANALYSIS
Session Chair: Ryan Kelly (Brigham Young University)
B405-407

TOC pm 02:30 **Large-Scale Top-Down Proteomics Across Two-Dozen Cell Types from Human Blood and Bone Marrow**; Rafael D Melani[1]; Robert V Gerbasi[1]; Jacek W Sikora[1]; Josiah E Hutton[1]; Jeannie M Camarillo[1]; Timothy Toby[1]; Kristina Srzentić[1]; Richard D Leduc[1]; Ryan T Fellers[1]; Joseph B Greer[1]; Andy I Kokaji[2]; Lissa C Anderson[3]; Christopher L. Hendrickson[3]; Paul M Thomas[1]; Neil L Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]STEMCELL Technologies Inc., Vancouver, BC; [3]NHMFL-FSU, Tallahassee, FL*

TOC pm 02:50 **Direct Mass Spectrometry Analysis of Protein Complexes and Intact Proteins Up to 70 kDa from Tissue**; Helen Cooper[1]; Rian Griffiths[1]; Albert Konijnenberg[2]; Rosa Viner[3]; *[1]University of Birmingham, Birmingham, United Kingdom; [2]Thermo Fisher Scientific, Eindhoven, Netherlands; [3]Thermo Fisher Scientific, San Jose, CA*

TOC pm 03:10 **Advancing High-Throughput Top-Down Analysis of Proteoforms up to 60 kDa using a Modified Orbitrap Tribrid Mass Spectrometer**; Michael W. Senko[1]; Romain Huguet[1]; Kristina Srzentić[2]; Vlad Zabrouskov[1]; Jesse D. Canterbury[1]; Christopher Mullen[1]; John E. P. Syka[1]; Luca Fornelli[3]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Cambridge, MA; [3]University of Oklahoma, Norman, OK*

TOC pm 03:30 **Capillary Zone Electrophoresis-Tandem Mass Spectrometry with Activated Ion Electron Transfer Dissociation and Ultraviolet Photodissociation for Large-Scale Top-Down Proteomics**; Eli McCool[1]; Jean Lodge[2]; Yansheng Liu[3]; Joshua J Coon[2]; Liangliang Sun[1]; *[1]Michigan State University, East Lansing; [2]University of Wisconsin, Madison, WI; [3]Yale University School of Medicine, West Haven, CT*

TOC pm 03:50 **Extending the Upper Mass Range Available to Top-Down Proteomics with 21 T-FTICR MS**; Lissa C. Anderson[1]; Chad R. Weisbrod[1]; David S. Butcher[1]; Christopher L. Hendrickson[1]; *[1]NHMFL-FSU, Tallahassee, FL*

TOC pm 04:10 **The Use of Top-Down Sequencing in the Evaluation of Enzyme Specificity of Streptococcal Cysteine Protease SpeB on Human IgG2**; Anja Resemann[1]; Waltraud Evers[1]; Robert Kane[2]; Fredrik Olsson[3]; Guillaume Tremintin[4]; Lars Vorwerg[1]; Detlev Suckau[1]; *[1]Bruker Daltonics, Bremen, Germany; [2]Bruker Daltonics Inc., Billerica, MA; [3]Genovis AB, Lund, Sweden; [4]Bruker Scientific, San Jose, CA*

2:30 - 4:30 pm Tuesday
DRUG TARGET IDENTIFICATION BY MS
Session Chair: Angela I. Calderon (Auburn University)
B302-305

TOD pm 02:30 **Proteome Wide Unbiased Target Identification for Radiation Mitigating Drug Candidate Using Thermal Proteome Profiling**; Kate Liu[1]; Constance Yuen[1]; William H. McBride[1]; Robert Damoiseaux[1]; Julian P. Whitelegge[1]; Joseph A. Loo[1]; *[1]UCLA, Los Angeles, CA*

TOD pm 02:50 **Development of a Novel Drug Target Identification Platform Based on Size (DTIPS)**; Yanting Guo[1]; Zhe Wang[1]; Dahang Yu[1]; Kellye A Cupp-Sutton[1]; Si Wu[1]; *[1]University of Oklahoma, Norman, OK*

TOD pm 03:10 **The Good, the Bad and the Ugly - Thermal Stability Changes for Targets, Off-Targets and Non-Targets of Small Molecule Drugs**; Alexey Chernobrovkin[1]; Cindy Caceres Körner[1]; Tomas Friman[1]; Johan Lengqvist[1]; Maria Thastrup[2]; Matilda Degn Vinther[2]; Daniel Martinez Molina[1]; *[1]Pelago Bioscience AB, Solna, Sweden; [2]Rigshospitalet, Copenhagen, Denmark*

TOD pm 03:30 **Integrative Mass Spectrometry and RNA-Sequencing Identifies DLK1 as a Candidate Immunotherapeutic Target in Neuroblastoma**; Amber K. Weiner[1,2]; Alexander B. Radaoui[2]; Simone Sidoli[1]; Karina L. Conkrite[2]; Zalman Vaksman[2]; Komal S. Rathi[2]; Pichai Raman[2]; Jo Lynne Harenza-Rokita[2]; Dan Martinez[2]; Tricia Bhatti[2]; Matthew Tsang[2]; Bruce Pawel[2]; Benjamin A. Garcia[1]; John M. Maris[1,2]; Sharon J. Diskin[1,2]; *[1]University of Pennsylvania, Philadelphia, PA; [2]Children's Hospital of Philadelphia, Philadelphia, PA*

TOD pm 03:50 **Mechanism and Dynamics of SAMT Analog Inactivation of HIV-1 Gag Polyprotein**; Lisa M. Miller Jenkins[1]; Elliott L. Paine[1]; Lalit Deshmukh[2,3]; Herman Nikolayevskiy[2]; Gaelyn C. Lyons[1]; John M. Louis[2]; Robert J. Gorelick[4]; David E. Ott[4]; G. Marius Clore[2]; Daniel H. Appella[2]; *[1]National Cancer Institute, Bethesda, MD; [2]National Institute of Diabetes and Digestive and Kidney Diseases, Bethesda, MD; [3]University of California San Diego, La Jolla, CA; [4]Frederick Nat'l Lab for Cancer Research, Frederick, MD*

TOD pm 04:10 **Illuminating the Druggable Proteome: Deconvolution of Drug Action by Multi-Omics, Thermal Profiling and High-Content Screening**; Doug Chapnick[1]; Christopher Ebmeier[1]; Kerri Ball[1]; Stephen Coleman[1]; Jeremy Jacobsen[1]; Kristofor Webb[1]; Travis Nemkov[2]; Xuedong Liu[1]; Michael Stowell[1]; Angelo D'Alessandro[2]; William Old[1]; *[1]University of Colorado Boulder, Boulder, CO; [2]University of Colorado, Denver - Anschutz, Aurora, CO*

2:30 - 4:30 pm Tuesday
FOOD SAFETY & CHEMISTRY: INNOVATIONS
Session Chair: Christine Fisher (US Food & Drug Administration)
B308-309

TOE pm 02:30 **Sensitive Multi-Mycotoxin Biomonitoring in Breast Milk by LC-MS/MS**; Dominik Braun[1]; Maximilian Eiser[1]; Doris Marko[1]; Benedikt Warth[1]; *[1]University of Vienna, Faculty of Chemistry, Department of Food Chemistry and Toxicology, Vienna, Austria*

TOE pm 02:50 **Formation of Toxic Iodinated Disinfection Byproducts during the Cooking of Pasta with Iodized Table Salt**; Huiyu Dong[1,2]; Ilona Nordhorn[1]; Karsten Lamann[1]; Danielle C. Westerman[1]; Hannah K Liberatore[1]; Susan D. Richardson[1]; *[1]University of*

South Carolina, Columbia, SC; [2]Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, Beijing, China

TOE pm 03:10 **Rapid Retrospective Assessment of Exposure of Cattle to Pesticides, Growth Promotors, Antibiotics by Use of In-House Developed Software Tools**; Marco Blokland[1]; Arjen Lommen[1]; Robin Wegh[1]; Frederike van Tricht[1]; Hans Mol[1]; Michel W.F. Nielen[1]; *[1]RIKILT, Wageningen, Netherlands*

TOE pm 03:30 **Utilization of the MasSpec Pen for Rapid and Direct Investigation of Meat Fraud**; Abigail Gatmaitan[1]; Jialing Zhang[1]; John Q. Lin[1]; Livia S Eberlin[1]; *[1]University of Texas, Department of Chemistry, Austin, TX*

TOE pm 03:50 **Ambient Ionization Coupled with a Miniature Mass Spectrometer for Rapid Analysis of Adulterated Additives in Food**; Xianshuang Meng[1]; Qiang Ma[1]; *[1]Chinese Academy of Inspection and Quarantine, Beijing, China*

TOE pm 04:10 **Innovations in Food Safety Assessment of Genetically Modified Crops – the Deregulation of a Sustainable Source of Omega-3 Oils**; Michelle Colgrave; *CSIRO, St Lucia, Australia*

2:30 - 4:30 pm Tuesday
CANCER RESEARCH
Session Chair: Erik Cressman (MD Anderson)
B312-314

TOF pm 02:30 **Proteomic Profiling of Cancer Cell Exosomes**; Kelly Servage[1]; Karoliina Stefanius[1]; Kim Orth[1]; *[1]UT Southwestern Medical Center, Dallas, TX*

TOF pm 02:50 **MALDI Detection of Exosomes for Cancer Studies**; Hubert H. Girault[1]; Yingdi Zhu[1]; *[1]Ecole Polytechnique Fédérale de Lausanne (EPFL), Sion, Switzerland*

TOF pm 03:10 **Live Single Cell Mass Spectrometry Reveals Cancer-Specific Metabolic Profiles of Circulating Tumor Cells**; Yasmine Abouleila[1]; Kaoru Onidani[2]; Ahmed Ali[1]; Eiso Hiyama[3]; Yoshihiro Shimizu[1]; Kazafumi Honda[2]; *[1]RIKEN, Osaka, Japan; [2]National Cancer Institute, Tokyo, Japan; [3]Hiroshima University, Hiroshima, Japan*

TOF pm 03:30 **Tumor and CD8 T Cells Metabolism and Consumption in the Tumor Microenvironment**; Lauranne Poncelet[1,2]; Rima Ait-Belkacem[1]; Pierre Levy[3]; Maarten Ligtenberg[3]; Daniel Peeper[3]; Jonathan Stauber[1]; *[1]Imabiotech, Loos, France; [2]Université de Lille, Lille, France; [3]Netherlands Cancer Insitute, Molecular oncology and Immunology department, Amsterdam, Netherlands; [4]ImaBiotech Corp, Boston, MA*

TOF pm 03:50 **Multisite Multimodal Mass Spectrometry Imaging of Organoids, Cell Extracts, and GEMMs to Explore Metabolic Changes in Colorectal Cancer Mutants**; Chelsea J Nikula[1]; Rory T. Steven[1]; Alex Dexter[1]; Efstathios A. Elia[1]; Teresa I. Murta[1]; Bin Yan[1]; Andrew D. Campbell[2]; Arafath K. Najumudeen[2]; Gregory Hamm[3]; David Gay[2]; Lucas Zeiger[2]; Aurelien Tripp[4]; Vincen Wu[5]; James S. McKenzie[5]; Paolo Inglese[5]; Jean-Luc Vorng[1]; Seyma Turkseven[5]; Simon Cameron[5]; Stefania Maneta-Stavrakaki[5]; Spencer A. Thomas[1]; Adam J. Taylor[1]; Ala Al-Afeef[1]; Tingting Fu[1]; Kenneth N. Robinson[1]; Weiwei Zhou[1]; Xavier Loizeau[1]; Ian S. Gilmore[1]; Richard J.A. Goodwin[3]; George Poulogiannis[4]; Zoltan Takats[5]; Owen J. Sansom[2]; Josephine Bunch[1,6]; *[1]National Physical Laboratory, London, United Kingdom; [2]Cancer Research UK Beatson Institute, Department of Invasion and Metastasis, University of Glasgow, United Kingdom; [3]AstraZeneca, iMED, United Kingdom; [4]Institute of Cancer Research, Division of Cancer Biology, United Kingdom; [5]Imperial College London, Department of Surgery and Cancer, United Kingdom*

TOF pm 04:10 **Interim Proteomic Analysis of Ovarian Cancer by the US Cancer Moonshot's Applied Proteogenomic OrganizationaL Learning and Outcomes (APOLLO) Program**; Nicholas Bateman[1,2]; Kathleen Darcy[1,2]; Emmanuel Petricoin[3]; Brian Hood[1]; Ming Zhao[4]; Kelly Conrads[1]; Christopher Tarney[1]; Christine Rojas[1]; Guisong Wang[1]; Craig Shriver[2]; Yovanni Casablanca[1,2]; George Larry Maxwell[1,2,4]; Thomas P. Conrads[1,2,4]; *[1]Gynecologic Cancer Center of Excellence, Annandale, VA; [2]John P. Murtha Cancer Center, Bethesda, MD; [3]Center for Applied Proteogenomics, George Mason University, Manassas, VA; [4]Inova Schar Cancer Institute, Annandale, VA*

2:30 - 4:30 pm Tuesday
INSTRUMENTATION: INNOVATIVE SEPARATIONS APPROACHES COUPLED TO MS
Session Chair: Xing-Fang Li (University of Alberta)
Auditorium, Bldg A

TOG pm 02:30 **The N-glycome Development Plan during Vertebrate Embryogenesis**; Yanyan Qu[1]; Zhenbin Zhang[1]; Michael Westphall[2]; Paul Huber[1]; Josh Coon[2]; Norman Dovichi[1]; *[1]University of Notre Dame, Notre Dame, IN; [2]University of Wisconsin, Madison, WI*

TOG pm 02:50 **Novel Capillary Columns for Bottom-Up and Top-Down Strategies Based Proteome Analysis**; Yu Liang[1]; Yutong Jing[2]; Lihua Zhang[1]; Yukui Zhang[1]; Ying Ge[2]; *[1]Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China; [2]University of Wisconsin, Madison, WI*

TOG pm 03:10 **Improved Sensitivity for Single Cell Proteomics Using micro-Chip Pillar Arrays**; Karl Mechtler[1,2]; Claudia Ctortecka[1,2]; Jeff Op Beck[3]; Paul Jacobs[3]; Gert Van Raemdonck[3]; Gabriela Krssakova[1,2]; Johannes Stadlmann[1,2]; *[1]Research Institute of Molecular Pathology (IMP), Vienna, Austria; [2]IMBA Institute of Molecular Biotechnology of the Austrian Academy of Sciences,, Vienna, Austria; [3]PharmaFluidics, Ghent, Belgium*

TOG pm 03:30 **Comprehensive Target and Non-Target Analysis of Unregulated Disinfection Byproducts with High Resolution Mass Spectrometry in Drinking Water**;Susana Y Kimura Hara[1]; Amy A. Cuthbertson[2]; Raphael Acabaya[1,3]; Cassiana Montagner Raimundo[3]; Susan D. Richardson[2]; *[1]University of Calgary, Calgary, AB; [2]University of South Carolina, Columbia, SC; [3]Campinas University, Campinas, Brazil*

TOG pm 03:50 **Coupling Advanced Chromatographic Methods for Analysis of Petroleum Products and Asphaltenes with On-line Detection by 21 T FT-ICR MS**; Jonathan Putman[1,2]; Donald F Smith[1]; Chad R. Weisbrod[1]; Steven M Rowland[1]; Martha L. Chacón-Patiño[1]; Yuri E. Corilo[1]; Greg T. Blakney[1]; Christopher L. Hendrickson[1,2]; Ryan P. Rodgers[1,2]; Alan G. Marshall[1,2]; *[1]National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; [2]Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL*

TOG pm 04:10 **High-Throughput Analysis of Phospholipid Isomers by Online Photochemical Derivatization and RPLC-MS**; Wenpeng Zhang[1,2]; Bing Shang[1,3]; Qinhua Chen[3]; Zheng Ouyang[4]; Yu Xia[1,2]; *[1]Department of Chemistry, Tsinghua University, Beijing, China; [2]Department of Chemistry, Purdue University, West Lafayette, IN 47907; [3]Affiliated Dongfeng Hospital, Hubei University of Medicine, Shiyan, China; [4]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instruments, Tsinghua University, Beijing, China*

2:30 - 4:30 pm Tuesday
ENERGY, PETROLEUM, AND BIOFUELS: INSTRUMENTATION AND APPLICATIONS
Session Chair: Amy McKenna
(National High Magnetic Field Laboratory)
A411-412

TOH pm 02:30 **Pseudo-Quantitative Approach for Molecular Nitrogen Compounds Analysis in Gas Oils and Vacuum Gas Oils Using FT-ICR/MS, GCxGC-NCD and GCxGC/HRMS**; Julie Guillemant[1]; Florian Albrieux[1]; Luis Pereira de Oliveira[1]; Marion Lacoue-Nègre[1]; Ludovic Duponchel[2]; Jean-François Joly[1]; *[1]Institut Francais du Petrole et Energies Nouvelles, Solaize, France; [2]LASIR, Lille, France*

TOH pm 02:50 **Extending the Application Range of a GC×GC High-Resolution TOF-MS platform for Fuel Analysis by Hyphenation to Thermal Analysis Techniques**; Uwe Kaefer[1,2]; Christopher Paul Rüger[2]; Thomas Gröger[1]; Mohammad Saraji-Bozorgzad[3]; Thomas Wilharm[4]; Ralf Zimmermann[1,2]; *[1]Joint Mass Spectrometry Centre, Comprehensive Molecular Analytics, Helmholtz Zentrum München, Neuherberg, Germany; [2]Joint Mass Spectrometry Centre, Chair of Analytical Chemistry, University of Rostock, Rostock, Germany; [3]Photonion GmbH, Schwerin, Germany; [4]ASG Analytik-Service Gesellschaft mbH, Neusäss, Germany*

TOH pm 03:10 **Case Studies in Oil Spill Forensics: Finding Petroleum Biomarkers with GCxGC-TOFMS**; Christina Kelly[1]; Joseph E Binkley[1]; Lorne M Fell[1]; Robert K Nelson[2]; Christopher M Reddy[2]; *[1]LECO Corporation, Saint Joseph, MI; [2]Woods Hole Oceanographic Institution, Woods Hole, MA*

TOH pm 03:30 **Structural Analysis of Compounds Refractory to the Hydrodenitrogenation Process of Heavy Oil Fractions by Ion Mobility Coupled with Mass Spectrometry**; Johann Le Maître[1,2]; Marie Hubert-Roux[1]; Benoit Paupy[2]; Sabrina Marceau[2]; Christopher Rüger[1]; Carlos Afonso[1]; Pierre Giusti[2]; *[1]Normandy University, COBRA laboratory, Mont Saint Aignan, France; [2]Total Research & Technology Gonfreville, Harfleur, France*

TOH pm 03:50 **Obtaining Tandem Mass Spectra of Individual Crude Oil Compounds within Narrow m/z Windows Using Cyclic Ion Mobility Mass Spectrometry**; Eunji Cho[1]; Eleanor Riches[2]; Martin Palmer[2]; Kevin Giles[2]; Jakub Ujma[2]; Yunju Cho[3]; Sunghwan Kim[1,3]; *[1]Kyungpook National University, Daegu, South Korea; [2]Waters Corporation, Wilmslow, United Kingdom; [3]Green-Nano Materials Research Center, Daegu, South Korea*

TOH pm 04:10 **Recent Developments in Petroleum Characterization by Advanced Chromatography and Mass Spectrometry**; Kuangnan Qian; *ExxonMobil Research Engineering, Annandale, NJ*

4:45-5:30 pm Tuesday
BIEMANN MEDAL LECTURE
Richard A. Yost (University of Florida), presiding
Murphy Ballroom, Bldg B, Level 5

Presentation of Research Award at Primarily Undergraduate Institution (PUI)

- Award sponsored by Agilent Technologies presented by Bryan Miller to Callie Cole (Fort Lewis College)

Presentation of the Research Awards

- Award sponsored by Bruker presented by Rohan A. Thakur to James F. Davies (University of California, Riverside).
- Award sponsored by Thermo Scientific presented by Iain Mylchreest to Nicolas L. Young (Baylor College of Medicine).
- Award sponsored by Waters Corporation presented by Lance Nicolaysen to Eleanor Browne (University of Colorado, Boulder)



Biemann Medal

Sarah Trimpin
Wayne State University

5:45 - 7:00 PM TUESDAY WORKSHOPS

There will be light refreshments in Building A foyers. All workshops are in Building A.

01 Top Down Proteomics: Advancing Widespread Adoption and Expanding Applications
(Top-Down Proteomics Interest Group)
Presiding: Nicolas Young, Frederik Lermyte
A402-403

Top-down protein mass spectrometry allows comprehensive characterization of proteoforms from complex mixtures and avoids many of the pitfalls associated with traditional bottom-up workflows. While the top-down approach is conceptually simple, a number of significant technical challenges must be overcome in order to successfully perform a top-down experiment. This combination of utility and difficulty has led to the creation and rapid expansion of the multinational Consortium for Top-Down Proteomics in 2012. In this workshop, we will bring together experienced and novice top-down mass spectrometry users in order to promote the development and democratization of these methods. The primary emphasis will be open discussion and debate. The selected topics and formal introductions will serve primarily to educate and provide greater accessibility to novice participants and induce discourse from a wide range of voices. We will discuss the following topics: Introduction to top-down proteomics and practical implementation in your laboratory; community initiatives and standardization; metrics for identification and accurate quantitation in biomedical research; and native mass spectrometry and native top-down proteomics. Each topic will be introduced by a 5-minute lightning talk, followed by approximately 10 minutes of audience discussion and debate. Thus, the majority of the workshop will be audience participation and a lively discussion amongst attendees. Contact workshop chairs if you are interested in presenting an introduction to spark the discussion of a topic.

02 Networking for Scientists: Celebrating Women Mass Spectrometrists (Year 2)
Presiding: Erin Baker, Anumita Saha
A404-405

In our second year of the Celebrating Women Mass Spectrometrists Workshop, we will utilize feedback from last year to refine our workshop. Due to the desire for more networking, this year we will start with a



There will be light refreshments in Building A foyers. All workshops are in Building A.

panel of ~6 women mass spectrometrists who have excelled in diverse careers in academia, industry and government. The session will kick off with panelists introducing themselves and giving a brief summary of their career paths. Then we will allow questions from the audience until there is ~30 min left in the workshop. At this time, the panelists will disperse in the room for one-on-one interaction with the audience. We feel this will give anyone who would like to attend, the chance to meet these women and ask them specific questions about their career paths in a social and non-threatening environment.

03 Say No to Drugs: Forensic Applications Outside of Traditional Illicit Drug Analysis
(Forensics & Homeland Security Interest Group)
Presiding: Christopher Mulligan, Brittany Casey
A406-407

As almost any chemical species could be potential evidence and/or a threat, given that it was involved in or alludes to criminal activities, the fields of forensic science and homeland security are some of the most demanding and comprehensive. To further complicate the issue, the large breadth of chemical targets can be found in various states of matter, as residues on many different substrates, or in the presence of complex chemical/biological matrices. Thus, forensic and security science has matured concurrently with advancements in analytical chemistry, and almost all processing of chemical substances incorporates some aspect of instrumental analysis.

Of the commonly-utilized instrumentation in these areas, mass spectrometry has a prominent role and is considered to be a "gold standard" technique (in the form of GC/MS) for illicit substance analysis. While much emphasis and effort (as evidenced by the recent Census of Publicly Funded Forensic Crime Laboratories by the Bureau of Justice Statistics) goes towards illicit drugs, the sensitivity and selectivity of MS-based methods are employed in many other areas of interest. This year, the workshop will move away from abused drugs to highlight other application areas of critical importance to forensic science and homeland security, such as chemical threats/CWAs, explosives/ firearms, toxicology, etc. Through discussions with a panel of scientists from the federal, private and academic sectors, the audience will gain insight into how researchers employ MS strategies in these important areas.

04 Proteoform Identification and Quantification Using Toppic Suite
Presiding: Xiaowen Liu, Si Wu, Liangliang Sun
A408

Top down mass spectrometry (MS) has gained increasing attention in the past decade because of its capability to sequence whole proteoforms with post-translational modifications (PTMs) and other alterations. Although many computational methods have been developed for top-down MS data analysis, it is still challenging for MS labs to efficiently identify and quantify proteoforms because of the complexity of the data and methods. TopPIC suite is an open source software package that is routinely used for proteoform identification and characterization by top-down MS. In this workshop, we will present the computational methods of the tools in TopPIC suite for spectral deconvolution and the identification of proteoforms with unknown alterations and those with multiple variable PTMS, and demonstrate new functions such as proteoform quantification and data visualization. We will give tutorials on applying the tools to various research problems ranging from phosphorylated proteoform identification to native proteomics. We will discuss with users and collect their feedback and suggestions for further improvement of the tools.

05 Protein Biomarkers Method Development & Validation by LCMS, HRMS and Hybrid LBA/LCMS: Recent Advancements
(Regulated Bioanalysis Interest Group)
Presiding: Jian Wang, Dian Su, Fabio Garofolo
A410

The 2019 Regulated Bioanalysis Interest Group (RBIG) Workshop is focused on recent advancements in protein biomarkers method development strategies and regulated Biomarker Assays Validation (BAV) by LCMS, HRMS and hybrid LBA/LCMS. This workshop will develop further mass spectrometry community discussions and consensus on the recently published recommendations on this topic including:

- Neubert, Song, Lee et al. - 2017 White Paper in Bioanalysis - https://www.future-science.com/doi/pdf/10.4155/bio-2017-4973
- Neubert, Olah, Lee et al. - 2018 White Paper in Bioanalysis - https://www.future-science.com/doi/pdf/10.4155/bio-2018-0285
- "[...]Accessibility and innovative integration of advanced technologies have accelerated the development of hybrid LBA/ LCMS, which has become an important bioanalytical platform to verify novel targets in discovery and confirm promising targets and biomarkers in early clinical development [...] Protein immunoaffinity techniques linked to MS (hybrid LBA/LCMS) have solidified their impact in translational research and in clinical analysis[...] This technique has been on an incredible journey in recent years that enabled growing adaptation through its use by an increasing number of practitioners and experts due to improved assay sensitivity and throughput, new reagents for capture approaches and automation of key steps, to name a few factors [...] Bioanalysts have advanced the ability from measuring soluble proteins to target engagement, moved from plasma to tissues including small biopsies, from soluble proteins to structural and membrane bound proteins and from concentration analysis to measuring protein synthesis rates." - excerpts from Bioanalysis (2017) 9(23) 1902-1903

Invited experts in this field will informally provide a wide range of perspectives on biomarkers method development and BAV by mass spectrometric techniques to stimulate an interactive & all-inclusive discussion with the audience

06 Improving Scientific Writing Skills
Presiding: Chris Petucci
A307

"The difference between the almost right word and the right word is really a large matter. It's the difference between the lightning bug and the lightning (Mark Twain)." A scientist's ability to clearly communicate ideas in written form has a major impact on his or her scientific reputation, obtaining grants, and publishing manuscripts. This workshop will be a hands-on session that includes essential grammar for scientists, writing grammatically correct sentences, and principles of logical paragraph development. At the conclusion of this workshop, you will have an increased knowledge of vital writing skills to prepare high quality manuscripts and other documents.

07 Metal Ions and Non-Threshold Ion Activation in Biomolecules
(Metal Ion Coordination Chemistry Interest Group)
Presiding: Franklin E. Leach III
A309

Biomolecular ions can interact with metal species in a variety of ways ranging from cofactors in metalloproteins to exchange with acidic protons. These interactions lead to structural changes that can be deduced by mass spectrometry and can affect the utility of specific MS/MS approaches to provide sufficient structural information. The workshop will focus on the application of non-threshold ion activation approaches (ExD, UVPD, CTD, etc.) to determine structure in biomolecules that interact with metal ions. Short presentations (~8-10 mins) from the community that demonstrate a fundamental understanding or unique application of these MS/MS approaches in



There will be light refreshments in Building A foyers. All workshops are in Building A.

metal ion systems will be given followed by time for discussion along with a series of lightning talks for any late breaking presentations of interest.

08 Protein Imaging - Are We There? Are All Issues Solved?
(Imaging MS Interest Group)
Presiding: Martina Marchetti-Deschmann, Peggi Angel
A311

MS Imaging allows to obtain detailed images of the spatial distribution of proteins in tissue and has tremendously progressed over the years. In this workshop experts will shortly introduce the participants to state-of-the-art protein imaging, covering aspects of specificity, dynamic range, protein identification and data interpretation. The speakers will foster discussions about potentials and limitations of protein imaging. This workshop is addressing everyone in the field, from beginners to experts and also those who are just interested in the method.

We moreover strongly encourage students and early stage researchers to give a short presentations (5 min/2-3 slides) on their perspectives of protein imaging, including insights or any challenges and limitations they face in this area. If you are interested in participating or have any questions, please contact us via email:
martina.marchetti-deschmann@tuwien.ac.at; angelp@musc.edu

09 Metabolomics: Points of Agreement and Disagreement
(Metabolomics Interest Group)
Presiding: Gary Patti, Jon Sobus
A312

The field of metabolomics emerged nearly twenty years ago, and targeted methods to measure metabolites were in place decades before. Given the tens of thousands of studies that are now available on metabolite profiling, there has been increasing clarity on best practices to quantitate small molecules with mass spectrometry. The purpose of this workshop is to review such analytical procedures, while also discussing practices in which disagreement persists. Moderators will first present themes from the literature representing perspectives they feel are widely shared by many researchers in the community. This will include sample preparation, metabolite extraction, and data processing steps. Focus will be dedicated to analytical strategies that may not have been agreed upon 10-15 years ago, but where progress has been made towards consensus. To contrast generally shared perspectives, moderators will also present views where varying opinions still exist among the community. Some examples may include: (i) what experimental data should constitute various confidence levels when identifying a metabolite? (ii) what are the minimal requirements for data sharing? (iii) how should databases be organized? Critical to the workshop will be the participation of the audience, whose input will help reflect the broader opinion of the community. At the end of the workshop, we hope participants will have a clearer sense of some basic ideas where there is general agreement and disagreement in the field of metabolomics.

10 Environmental MS: Detection of Emerging Contaminants
(Environmental Applications Interest Group)
Presiding: Chris Gill
A313

New classes of compounds and contaminants emerge every decade, encouraging analytical scientists to come up with state-of-the-art methodologies for their analysis. New instrumentation in mass spectrometry is driving the field of unequivocal identification (accurate mass techniques) and lower detection limits (super sensitive instrumentation). This workshop will be focused broadly on discussing the best techniques and analytical approaches, including sample preparation, for the determination of important emerging contaminants that require generation of new methods, such as nanoparticles, microplastics and perfluorinated compounds (PFOS/PFOA). Presentations will be limited to briefly introduce the topic to prioritize active discussion among environmental scientists.

11 Visualization, Comparison and Accessibility of Large Data Sets
(Analytical Lab Managers Interest Group)
Presiding: David Quilici, Samuel Mackintosh
A314

Analytical laboratories face significant challenges related to the analysis and storage of large data sets on behalf of principal investigators, many of whom have little experience with data analysis themselves. These investigators need to be able to understand what they are looking at, search their data easily, and extract useful information. In addition, analytical labs have the responsibility to maintain consistent standards for data analysis and to store and share large data sets appropriately and economically. The 2019 ASMS Analytical Lab Managers Workshop will focus on potential solutions to some of these challenges. Specifically, the workshop will cover data visualization techniques, standards for data normalization and comparison, and approaches to data storage and sharing. Three fifteen-minute presentations will be given, with each talk followed by a ten-minute discussion period.

12 Advances in Polymer Mass Spectrometry - Architecture
(Polymeric Materials Interest Group)
Presiding: Christina Mastromatteo, Jessica Hoskins
A315

This year's meeting will consist of three distinct sections; a workshop, student poster elevator talks, and an open forum.

To start with, we will have two short tutorials on analysis of polymer architecture:

- KMD applications to polymer analysis
- Hydrogel crosslinking studied by mass spectrometry

Secondly, we will host a series of short Polymer Section poster presentations (3-5 min each) by any students / presenters regarding their upcoming posters. This will provide each presenter an opportunity to promote their work externally to a professional scientific audience in their specialized field.

There will then be an open forum, in which attendees are invited to ask about any particular issues or questions that they would like to ask for help with. In addition, input will be sought for future Workshop topics.

13 (Emotional) Intelligence Gathering
(Career Development Interest Group)
Presiding: Lucinda Hittle, Charles Veltri
A316

Have you ever wondered how to improve your ability to think on your feet, resolve conflicts with others, and manage your emotions more effectively? Emotional intelligence may be one of the most underestimated elements of a successful career. This workshop will take participants through a brief assessment of their emotional intelligence quotient (EQ) then break out into small group discussions facilitated by veteran scientists across diverse sectors including industry, government and non-profit agencies, and academia. The goals of this workshop will be to foster relationships across the society that span the boundaries of geography, age, level of experience, and academic training as well as enabling networking and small group discussions. No experience required, but imagination and an open mind are pre-requisites!

14 MS in Extractable and Leachable Analysis
Presiding: Kate Comstock, Gyorgy Vas
A303

Mass spectrometry plays an essential role in extractable and leachable (E&L) analysis. Complete E&L profiles require GC-MS, LC-MS, and ICP-MS analysis. The advancements in mass spectrometry instrumentation and new techniques provide new and much-needed tools for confident and comprehensive E&L profiling.



There will be light refreshments in Building A foyers. All workshops are in Building A.

Currently, the increasing demands for E&L analysis are driven by growth in medical devices, single-use systems (SUS), continuous processing in bioproduction, etc. The variation in materials, applications, and interactions with contact media of these products pose new challenges for E&L analysis. Furthermore, the existing E&L regulations are lacking in clarification of acceptance for these new products.

There are many techniques and new developments for E&L analysis in terms of sample preparations, chromatographic separations, and data acquisitions by various mass spectrometry instruments. In addition, the data processing and interpretation often are rate-limiting factors, and there is an urgent need for efficient, easy-to-use data processing software, E&L database and spectral libraries, and result reports generator.

This workshop will provide a venue for E&L analysis scientists to discuss all the above issues, exchange practices, also present problems and challenges concerning mass spectrometry instrumentation, methodologies, and data processing. Through this workshop, E&L scientists will have direct open discussion and information exchange, establish and expand networks. It will promote good science and advancement of mass spectrometer's usage in E&L analysis.

15 HDX, Covalent Labeling & Cross-Linking: Status of Community-Initiatives and New Developments and Applications
(HDX Covalent Labeling & Cross Linking Interest Group)
Presiding: Kasper Rand, Jim Bruce

Recent innovations in MS instrumentation, sample preparation strategies, cross-linking and chemical labeling reagents, and bioinformatics tools have significantly facilitated the developments and applications of HDX, covalent labeling and cross-linking approaches in protein structural and interaction analysis. In order to allow robust data evaluation and result comparison among experiments and across laboratories, data acquisition, analysis and interpretation need to be standardized. Since the last workshop, community-wide efforts have focused on these topics and in the first part of the workshop, one panelist from each community will present current status and highlights from this work for the benefit of beginners and experts alike. In addition, interactive discussions among audience members will be stimulated by the panelists, regarding to future perspectives for other topics that need to be harmonized within each fields. The second part of the workshop will focus on most recent technical developments or new areas of application within HDX/XL/CL-MS. Exciting and promising new developments will be highlighted by 5 min talks from invited members of the community, with a focus on current applicability and limitations. The invited speakers will form a panel for this second part of the workshop and there will be ample time for questions and answers including an opportunity for novices/students to contribute anonymous questions on fundamentals.

16 Lipidomics: Path to Clinical Utility
(Lipids & Lipodomics Interest Group)
Presiding: John Bowden, Kim Ekroos,
A301

The field of lipidomics is rapidly evolving, driven by high expectation in its ability to afford new opportunities for studying lipids in health and disease and in many other fields of research. As such, in this lipidomics workshop, we aim to discuss the current status of lipidomics in the clinical arena. The workshop will be designed to stimulate discussion on several key questions, including: what are the current roadblocks preventing the universal adaptation of lipidomics in the clinical setting, which lipids/disease states already show clinical promise and which should we be focusing on next, and moving forward within the clinic, how much effort should be placed on those lipids that are historically difficult to measure but might have clinical promise? At present, the field is currently challenged by large disparities in methodologies and technologies and in how users apply them, resulting in an increasing number of publications of varying quality. Two potential reasons for this are the lack of a common language and the lack of community-accepted best practice guidelines, both stalling the future development and true utilization of lipidomics in clinical research and diagnostics. This workshop will review the current challenges and discuss strategies moving forward, including the community-wide harmonization (and standardization) of lipidomics. A group of experts will share their experience and answer any questions, and views from the audience will be discussed.

17 Data Independent Acquisition: Expanding the Scope of DIA Strategies for Quantitative Mass Spectrometry
(Data Independent Acquisition Interest Group)
Presiding: Hannes Röst, Birgit Schilling
A305

In quantitative proteomics, the fundamental aim is to accurately identify and quantify analytes across various conditions. Data independent acquisition (DIA) has recently emerged as a promising method to accurately quantify analytes in complex samples, allowing consistent detection and quantification of thousands of proteins across large sample cohorts. Utilizing MS2-based quantification (as in SRM/PRM) in high throughput workflows (as in DDA) has led to impressive results with highly consistent and accurate quantitative data matrices suitable for systems biology, systems medicine and personalized medicine applications. However, most current methods focus on accurate protein quantification using a label-free approach. However, the DIA approach can readily be applied to other MS-based questions and can be beneficial if high-quality fragment ion data is essential for correct analyte characterization. This workshop will discuss novel technological and software innovations in the field of DIA: How can novel advances in computer science (deep learning) advance the field of DIA and which novel analysis methods do they make available? What specific challenges await when expanding the scope of DIA beyond unmodified peptides (PTMs, SAV, lipids, small molecules)? How can ion mobility be integrated with DIA? How can very short gradients be exploited in DIA? This workshop will focus on existing and emerging approaches using novel technology and software in DIA and discuss some unique challenges, and opportunities, of translating the recently developed DIA approaches (such as targeted extraction) to these fields.

18 Trans-Proteomic Pipeline: Recent Advances and Future Directions
Presiding: Luis Mendoza, David Shteynberg, Eric Deutsch
A304

The workshop will begin with a brief overview of the Trans-Proteomic Pipeline (TPP) and its newest features and capabilities. We will then focus on four individual topics, fostering a discussion with workshop participants on the current strengths, weaknesses, and future directions for the TPP. The workshop will enable participants to describe challenges in proteomic data analysis and help drive directions in software approaches through needs of the community. The topic leads for discussion are: proteogenomics & PEFF applications, analyzing PTMs with PTMProphet, cross-linking analysis with Kojak 2.0, and deploying the TPP using Docker containers & cloud computing platforms. Each topic will be introduced with a brief summary of features and ideas. Then feedback and discussion by the workshop participants will be promoted.



From 7:00 am Wednesday
CORPORATE BREAKFAST SEMINARS
CONVENTION CENTER AND OMNI CNN CENTER HOTEL
See page 16 for detailed schedule. Reservation or RSVP required.

8:30 - 10:30 am Wednesday
METABOLOMICS: NEW TECHNOLOGIES AND APPLICATIONS
Session Chair: Nichole Reisdorph (University of Colorado Anschutz Medical Campus)
Murphy Ballroom, Bldg B, Level 5

WOA am 08:30 **Uncovering the Role of Autophagy Impairment on Dysregulated Lipid Metabolism in Skeletal Muscle Aging through Multi-Platform Metabolomics Analysis**; Christian Toonstra[1]; Zoe Maxwell[1]; Heather Brown[1]; Michelle Kuhns[1]; Edgar Arriaga[1]; *[1]University of Minnesota, Minneapolis, MN*

WOA am 08:50 **Metabolically Labeled Ribonucleotides Enable Multiplexed Quantitative Analysis of the Effects of Stress and Viral Infection by High Resolution Mass Spectrometry**; Thomas J Kenderdine[1]; Reza Nemati[2]; Rachel Netzband[1,3]; Molly FitzGibbon[4]; Will McIntyre[1]; Cara T. Pager[1,3]; Daniele Fabris[1,3]; *[1]SUNY Albany, Albany, NY; [2]Biogen, Cambridge, MA; [3]The RNA Institute, University at Albany, Albany, NY; [4]University of California, San Diego, CA*

WOA am 09:10 **Native ESI-MS Based Metabolomics Enables the Search for Metal-Binding Molecules**; Allegra Aron[1,2]; Daniel Petras[2,3,4]; Julia M Gauglitz[1,2]; Hui Zhi[5]; Manuela Raffatellu[2,5,6]; Pieter C. Dorrestein[1,3]; *[1]University of California San Diego, Collaborative Mass Spectrometry Innovation Center, La Jolla, CA; [2]University of California San Diego, Center for Microbiome Innovation, La Jolla, CA; [3]University of California San Diego, Collaborative Mass Spectrometry Innovation Center, La Jolla, CA; [4]University of California San Diego, Scripps Institution of Oceanography, La Jolla, CA; [5]University of California San Diego Division of Host–Microbe Systems & Therapeutics, Department of Pediatrics, La Jolla, CA; [6]Chiba University–University of California San Diego Center for Mucosal Immunology, Allergy, and Vaccines (CU-UCSD cMAV), La Jolla, CA*

WOA am 09:30 **Creation and Annotation of a Recurrent Spectral Library of Cho Cell Metabolites and Media Components**; Kelly H. Telu[1]; Ramesh Marupaka[1]; Nirina R. Andriamaharavo[1]; Yamil Simón-Manso[1]; Yuxue Liang[1]; Yuri A. Mirokhin[1]; Xinjian Yan[1]; Tallat H. Bukhari[1]; Stephen E. Stein[1]; *[1]NIST, Gaithersburg, MD*

WOA am 09:50 **Quantitative Sub-Cellular acyl-CoA Analysis Using SILEC Internal Standards**; Sophie Trefely[1]; Katharina Huber[2]; Joyce Liu[2]; Mary Doan[3]; Helen Jiang[3]; Jay Singh[3]; Kenneth C Bedi[2]; J. Eduardo Rame[2]; Kathryn E. Wellen[2]; Nathaniel W Snyder[3]; *[1]University of Pennsylvania, Philadelphia, PA; [2]University of Pennsylvania, Philadephia, PA; [3]Drexel University, Philadelphia, PA*

WOA am 10:10 **Chemical Isotope Labeling LC-MS for Studying the Metabolic Response of Single Cells to Heat Shock**; Wan Chan[1]; Michael C. Schultz[1]; Liang Li[1]; *[1]University of Alberta, Edmonton*

8:30 - 10:30 am Wednesday
CARBOHYDRATES
Session Chair: Ron Orlando (University of Georgia)
B401-402

WOB am 08:30 **CUPRA-ZYME: A Novel ESI-MS Method for Measuring Carbohydrate-Active Enzyme Activities and Profiling their Substrate Specificities**; Zhixiong Li[1]; Pavel I Kitov[1]; Erick Bolivar[1]; Elena N Kitova[1]; John Klassen[1]; *[1]Department of Chemistry, University of Alberta, Edmonton, AB*

WOB am 08:50 **Analysis of N-Glycans Released from Monoclonal Antibodies by Combining Ultra High-Resolution Ion Mobility Spectrometry and Cryogenic Ion Spectroscopy**; Natalia Yalovenko[1]; Ahmed Ben faleh[1]; Stephan Warnke[1]; Thomas R. Rizzo[1]; *[1]Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*

WOB am 09:10 **Dissecting Fragment Ion Structures of Protonated Oligosaccharides by MSn, Ion Mobility Spectrometry, and Gas-Phase Hydrogen/Deuterium Exchange Mass Spectrometry**; Abhigya Mookherjee[1]; Sanjit Singh Uppal[1]; Miklos Guttman[1]; *[1]University of Washington, Seattle, WA*

WOB am 09:30 **A Simplified Approach to N-Glycan Profiling of Cultured Cells Using MALDI Imaging Mass Spectrometry**; Janet Saunders[1]; Cassandra L Clift[1]; Anand S. Mehta[1]; Richard R. Drake[1]; Peggi Angel[1]; *[1]Medical University of South Carolina, Charleston, SC*

WOB am 09:50 **Comparison of Charge Transfer Dissociation (CTD) and Electron Detachment Dissociation (EDD) for the Structural Analysis of Glycosaminogylcans**; Lauren Pepi[1]; Zachary J Sasiene[2]; Praneeth M Mendis[2]; Glen P Jackson[2,3]; I. Jonathan Amster[1]; *[1]University of Georgia, Athens, GA; [2]West Virginia University.C. Eugene Bennett Department of Chemistry, Morgantown, WV; [3]Department of Forensic and Investigative Science, West Virginia University, Morgantown, WV*

WOB am 10:10 **NanoPGC-LC–EED-MS/MS Analysis of N-linked Glycans in Human Serum**; Yang Tang[1]; Juan Wei[1]; Catherine E. Costello[1]; Cheng Lin[1]; *[1]Boston University, Boston, MA*

8:30 - 10:30 am Wednesday
FUNDAMENTALS FOR EVERYONE: PEPTIDES AND PROTEINS
Session Chair: Cheryl Lichti (Washington University in St. Louis)
B405-407

WOC am 08:30 **Robust Methods for Endogenous Proteoform Characterization by Immunoprecipitation and Subsequent Targeted Top-Down Proteomic Analysis**; Caroline DeHart[1]; Luca Fornelli[2]; Lauren M Adams[3]; Jacek W Sikora[1]; Vincent Gerbasi[1]; Ryan T Fellers[1]; Richard D Leduc[1]; Paul M Thomas[1]; Philip D. Compton[1]; Neil L Kelleher[1]; *[1]Proteomics Center of Excellence, Northwestern University, Evanston, IL; [2]University of Oklahoma, Norman, OK; [3]Northwestern University, Evanston, IL*

WOC am 08:50 **Ion Mobility Separations of Proteins at Extreme Fields with Dipole Alignment Tunable by Changing the Gas Pressure**; Alexandre A. Shvartsburg[1]; Roch Andrzejewski[2]; Andrew Entwistle[2]; Roger Giles[2]; *[1]Wichita State University, Wichita, KS; [2]Shimadzu Corporation, Manchester, United Kingdom*

WOC am 09:10 **Nanodroplet Sample Processing, Ultra-Low-Flow nanoLC and Next-Generation Tribrid MS Enable In-Depth, Label-Free Profiling of Single Mammalian Cells**; Yongzheng Cong[1]; Ying Zhu[2]; Yiran Liang[1]; Maowei Dou[2]; Greg Foster[3]; Daniel Lopez-Ferrer[3]; Yufeng Shen[4]; Ryan T. Kelly[1,2]; *[1]Brigham Young University, Provo, UT; [2]Pacific Northwest National Laboratory, Richland, WA; [3]Thermo Fisher Scientific, San Jose, CA; [4]CoAnn Technologies, LLC, Richland, WA*

WOC am 09:30 **FAIMS Enables Increased Proteome Coverage on a Q Exactive Platform with Short LC Gradients**; Dorte Breinholdt Bekker-Jensen[1]; Patrick L. Ruether[2]; Christian D. Kelstrup[2]; Jesper V. Olsen[2]; *[1]University of Copenhagen, NNF CPR, Copenhagen N, Denmark; [2]University of Copenhagen NNF CPR, Copenhagen N, Denmark*

WOC am 09:50 **Multimodal Approaches for Non-targeted Discovery of Endogenous D-amino Acid Containing Peptides**; David H. Mast[1]; James W. Checco[1]; Elena V. Romanova[1]; Jonathan V. Sweedler[1]; *[1]University of Illinois at Urbana Champaign, Urbana, IL*

WOC am 10:10 **Two Dimensional Mass Spectrometry (2DMS) – the Next Dimension in Proteomics**; Pui Yiu Lam[1]; Christopher A. Wootton[1]; Kung Ching Cookson Chiu[1]; Tomos E. Morgan[1]; Remy Gavard[1]; Meng Li[1]; Mark P. Barrow[1]; Peter B. O'Connor[1]; *[1]University of Warwick, Coventry, United Kingdom*

8:30 - 10:30 am Wednesday
MICRODOSING AND MICROSAMPLING: ANALYTICAL CHALLENGES
Session Chair: Uliana Danilenko (CDC)
B302-305

WOD am 08:30 **Rapid, Untargeted Metabolomic Profiling of Single Cells in Their Native Environment Using Single-Cell Printer-Liquid Vortex Capture-Mass Spectrometry**; John F. Cahill[1]; Julian Riba[2,3]; Vilmos Kertesz[1]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN; [2]University of Freiburg, 79110, Germany; [3]Cytena GmbH, 79108, Germany*

WOD am 08:50 **"Dip and Go": High-Throughput Direct Bioassays by Inductive nESI**; Zhenwei Wei[1]; Zhuoer Xie[1]; Reshma Kuvelkar[2]; Vinit Shah[2]; Kevin P. Bateman[2]; David G. McLaren[2]; Graham R. Cooks[1]; *[1]Purdue University, West Lafayette, IN; [2]Merck & Co. Inc., Kenilworth, NJ*

WOD am 09:10 **High Speed System for Analysis of Biological Samples that Corrects for ESI Ionization Suppression in Real Time**; Thomas R. Covey[1]; Peter Kovarik[1]; Chang Liu[1]; *[1]SCIEX, Concord, ON*

WOD am 09:30 **On-Line Spatially Resolved Surfaces Sampling Capillary Electrophoresis Mass Spectrometry**; Ingela Lanekoff[1]; Kyle D Duncan[1]; *[1]Uppsala University, Uppsala, Sweden*

WOD am 09:50 **Inter-Laboratory Validation of Solid-Phase Microextraction-Based Protocol for Untargeted Profiling of Lipids in Rat Brain**; Mariola Olkowicz[1]; Cian Monnin[2]; Nathaly Reyes-Garcés[1,3]; Sofia Lendor[1]; Ezel Bojaci[1,4]; Miao Yu[1,5]; German Augusto Gomez-Rios[1,3]; Clement Hamani[6]; Barbara Bojko[1,7]; Dajana Vuckovic[2]; Janusz Pawliszyn[1]; *[1]University of Waterloo, Waterloo, ON; [2]Concordia University, Montreal, Qc; [3]Restek Corporation, Bellefonte, PA; [4]Department of Chemistry, Middle East Technical University, Ankara, Turkey; [5]Icahn School of Medicine at Mount Sinai, New York, NY; [6]Sunnybrook Health Sciences Centre, Toronto, ON; [7]Nicolaus Copernicus University, Torun, Poland*

WOD am 10:10 **Controlling Variance for Self-collected Plasma; Anatomy, Analysis and Accuracy**; Russell Grant[1]; Bradley Collier[1]; Jennifer Pollock[1]; Julia Hannon[1]; Matthew Crawford[1]; *[1]Labcorp., Burlington, NC*

8:30 - 10:30 am Wednesday
ENVIRONMENTAL: INNOVATIVE APPROACHES AND INSTRUMENTATION
Session Chair: Pierangela Palma (University of Urbino)
B308-309

WOE am 08:30 **Mass Spectrometry of Single Picoliter Droplets to Explore the Chemistry of Atmospheric Aerosol**; James F Davies; *UC Riverside, Riverside, CA*

WOE am 08:50 **Byproducts Formation in a VOC Air Cleaning System: Real-Time Analysis Using a Compact FTICR in a Model Plasma Reactor**; Sébastien Thomas[1]; Nicole Blin-Simiand[2]; Joel Lemaire[3]; Michel Héninger[3]; Hélène Mestdagh[3]; Lionel Magne[2]; Stéphane Pasquiers[2]; Essyllt Louarn[4]; *[1]CSNSM – CSNCM - UMR8609 – Univ. Paris-Sud, CNRS, Univ. Paris-Saclay, Orsay, France; [2]LPGP - UMR8578 - Univ. Paris-Sud, CNRS, Univ. Paris-Saclay, Orsay, France; [3]LCP - UMR8000 - Univ. Paris-Sud, CNRS, Univ. Paris-Saclay - Orsay, Orsay, France; [4]LCP - UMR8000 - Univ. Paris-Sud, CNRS, Univ. Paris-Saclay, Orsay, France*

WOE am 09:10 **MALDI-TOF Imaging and LC-HRMS: New tools for Degradation Studies of Polymer Probes Exposed to Different Waste Water Environments**; Damia Barcelo[1]; Antoni Ginebreda[1]; Maria Vila Costa[1]; Bozo Zonja[1]; Nicola Montemurro[1]; A Martinez Varela[1]; Sandra Perez[1]; Daniel Rivas[1]; *[1]IDAEA-CSIC, Barcelona, Spain*

WOE am 09:30 **Iodinated X-ray Contrast Media as a Source of Iodine for the Formation of Iodinated DBPs upon Chlorination during Wastewater Treatment**; Caroline O. Granger[1]; Hannah K. Liberatore[1]; Susan D. Richardson[1]; Mark Ferrey[2]; *[1]University of South Carolina, Columbia, SC; [2]Minnesota Pollution Control Agency, St. Paul, Minnesota*

WOE am 09:50 **Dissolved Organic Matter Molecular Composition to Optical Properties Relations as Determined by Ultra-High Resolution Mass-Spectrometry**; Alexander Zherebker[1]; Evgeny Shirshin[2]; Oleg Kharybin[1]; Irina Perminova[2]; Eugene (evgeny) Nikolaev[1]; *[1]Skolkovo institute of science and technology, Moscow Region, Russian Federation; [2]Moscow State University, Moscow, Russian Federation*

WOE am 10:10 **Chemical or Electron Ionization? The Application of GC×GC HRT in Environmental Research with Source-Specific Molecular Markers**; Ulrich M Hanke[1]; Robert K Nelson[1]; Christina Kelly[2]; Bruno Glaser[3]; Christopher M Reddy[1]; *[1]Woods Hole Oceanographic Institution, Woods Hole, MA; [2]LECO Corporation, St Joseph, MI; [3]Martin-Luther-University Halle-Wittenberg, Halle / Saale, Germany*

8:30 - 10:30 am Wednesday
ION MOBILITY: NEW DEVELOPMENTS & APPLICATIONS
Session Chair: Helen Cooper (University of Birmingham)
B312-314

WOF am 08:30 **Segmented Ion Fractionation and High Field Asymmetric Waveform Ion Mobility Spectrometry Expands Proteome Coverage to Uncover Sequence Variants**; Eric Bonneil[1]; Sibylle Pfammatter[1,2]; Pierre Thibault[1,2]; *[1]IRIC-Université de Montréal, Montréal, QC; [2]Department of Chemistry, Université de Montréal, Montréal, QC*

WOF am 08:50 **A Novel Cyclic Ion Mobility Enabled Method for Data Enrichment, Selectivity and Sensitivity Enhancement in MS/MS Experiments**; Eleanor Riches[1]; Martin Palmer[1]; Jakub Ujma[1]; Kevin Giles[1];

Sunghwan Kim[2]; [1]*Waters Corporation, Wilmslow, United Kingdom;* [2]*Kyungpook National University, Daegu, South Korea*

WOF am 09:10 **A Drift-Tube Ion Mobility-Mass Spectrometer for Native Mass Spectrometry: High Resolution Ion Mobility, Collision Induced Unfolding, and Electron Capture Dissociation**; Varun Gadkari[1]; Ruwan T Kurulugama[2]; John C. Fjeldsted[2]; Brandon T. Ruotolo[1]; [1]*University of Michigan, Ann Arbor, MI;* [2]*Agilent Technologies, Inc., Santa Clara, CA*

WOF am 09:30 **Top-Down Sequencing of Mobility-Selected Glycoprotein Complexes Using Tandem Trapped Ion Mobility Spectrometry – Mass Spectrometry (Tandem-TIMS/MS)**; Fanny C Liu[1]; Mark E. Ridgeway[2]; Melvin A. Park[2]; Christian Bleiholder[1]; [1]*Florida State University, Tallahassee, FL;* [2]*Bruker Daltonics Inc., Billerica, MA*

WOF am 09:50 **Trapped Ion Mobility Mass Spectrometry as a Tool for Neuropeptidome Analysis**; Geert Baggerman[1,2]; Kristina Marx[3]; Harshavardhan Budamgunta[2]; Gerben Menschaert[4]; Kurt Boonen[2,5]; [1]*Vito, Mol, Belgium;* [2]*Uantwerpen, Antwerpen, Belgium;* [3]*Bruker Daltonik GmbH, Bremen, Germany;* [4]*UGent, Gent, Belgium;* [5]*Vito, Mol, Belgium*

WOF am 10:10 **Broad Targeted Phosphoproteomics analysis Using Structures for Lossless Ion Manipulations (SLIM) Ion Mobility-MS**; Yi-Ting Wang[1]; Gabe Nagy[1]; Adam Hollerbach[1]; Chia-Feng Tsai[1]; Karin Rodland[1]; Tujin Shi[1]; Richard Smith[1]; Tao Liu[1]; [1]*Biological Science Division, Pacific Northwest National Laboratory, Richland, WA*

8:30 - 10:30 am Wednesday
FUNDAMENTALS FOR EVERYONE: STRUCTURAL ELUCIDATION
Session Chair: Albert T. Lebedev (Moscow State University)
Auditorium, Bldg A

WOG am 08:30 **Structural Elucidation of Metabolites Using Accurately Computed Fragmentation Patterns and Searches in Databases of 2D Molecular Structures**; Bela Paizs[1,2]; Zoltan Takats[2,3]; [1]*Bangor University, Bangor, United Kingdom;* [2]*deshape ltd, Bangor, United Kingdom;* [3]*Imperial College, London, United Kingdom*

WOG am 08:50 **Gas-Phase Ion/Ion Chemistry for the Detailed Structural Analysis and Relative Quantitation of Unsaturated Lipids**; Caitlin E. Randolph[1]; David J. Foreman[1]; Stephen J. Blanksby[2]; Scott A McLuckey[1]; [1]*Purdue University, West Lafayette, IN;* [2]*Central Analytical Research Facility, Institute for Future Environments, Queensland University of Technology, Brisbane, Australia*

WOG am 09:10 **IRMPD Ion Spectroscopy and Ion-Molecule Reactions as Structure Elucidation Tools for Peptide Radical Ions**; Victor Ryzhov; *Northern Illinois University, Dekalb, IL*

WOG am 09:30 **Characterization of Small Molecule Unknowns Using the AcquireX Data Acquisition Strategy**; Seema Sharma[1]; Stephanie N. Samra[1]; Caroline Ding[1]; Kate J. Comstock[1]; Reiko Kiyonami[1]; Scott M. Peterman[1]; Graeme McAlister[1]; Mark Sanders[1]; Vlad Zabrouskov[1]; [1]*Thermo Fisher Scientific, San Jose, CA*

WOG am 09:50 **Cationized Glycan Fragmentation Chemistry**; Benjamin Bythell; *Univ. of Missouri-St. Louis, St. Louis, MO*

WOG am 10:10 **Comparative Study of 'Ortho–' and 'Para–' Effects in EI Spectra Of Silyl, Acyl, Mesyl and Tosyl Derivatives of tert-Butylphenols / Thiophenols**; Anzor Mikaia[1]; Nino Todua[1,2]; Levan Megutnishvili[1]; [1]*National Institute of Standards and Technology, Gaithersburg, MD;* [2]*Strativia, Largo, MD*

8:30 - 10:30 am Wednesday
SYNTHETIC POLYMERS
Session Chair: Rainey Patterson Garland (Eastman Chemical Co.)
A411-412

WOH am 08:30 **High-Throughput Screening of Polysorbates by High Resolution Mass Spectrometry with Rapid H/D Exchange**; Kui Yang[1]; Asha Hewarathna[1]; Ilan Geerlof-Vidavsky[1]; Connie Ruzicka[1]; David Keire[1]; [1]*FDA, St. Louis, MO*

WOH am 08:50 **Analysis of Biocompatible Synthetic Polymers with Electron Capture Dissociation and Two-Dimensional Mass Spectrometry**; Tomos E. Morgan[1]; Sean H. Ellacott[1]; Andrew Kerr[1]; Christopher A. Wootton[1]; Bryan P. Marzullo[1]; Maria van Agthoven[1]; Mark P. Barrow[1]; Anthony W. T. Bristow[2]; Sebastien Perrier[1]; Peter B. O'Connor[1]; [1]*University of Warwick, Coventry, United Kingdom;* [2]*AstraZeneca, Macclesfield, United Kingdom*

WOH am 09:10 **Probing the Reaction Mechanisms of Troger's Base Polymers of Intrinsic Microporosity**; Anthony P. Gies[1]; Robert E. Hefner[1]; Nathan J. Rau[1]; Praveenkumar Boopalachandran[1]; [1]*The Dow Chemical Company, Lake Jackson, TX*

WOH am 09:30 **Secured Communications with Sequence-Controlled Synthetic Polymers: Decoding by Tandem Mass Spectrometry, Decrypting by Ion Mobility Spectrometry**; Jean-Arthur Amalian[1]; Gianni Cavallo[2]; Abdelaziz Al Ouahabi[2]; Jean-François Lutz[2]; Laurence Charles[1]; [1]*Aix-Marseille University, Marseille Cedex 20, France;* [2]*Institut Charles Sadron, University of Strasbourg, Strasbourg, France*

WOH am 09:50 **Determination of Gas Phase Ion Structures of Polar Homopolymers through Ultra-High Resolution Ion Mobility Spectrometry-Mass Spectrometry**; Xi Chen[1,2]; Shannon A. Raab[3]; Timothy Poe[1]; David E. Clemmer[3]; Carlos Larriba Andaluz[1]; [1]*IUPUI, Indianapolis, IN;* [2]*Purdue University, West Lafayette, IN;* [3]*Indiana University, Bloomington, IN*

WOH am 10:10 **Charge Detection Mass Spectrometry with an Orbitrap Analyzer**; Jared O. Kafader[1]; Rafael D. Melani[1]; Bryan P. Early[1]; Kenneth R. Durbin[1]; Neil L. Kelleher[1]; Philip D. Compton[1]; Steven C. Beu[2]; Deven L. Shinholt[3]; Joshua T. Maze[3]; Alexander A. Makarov[4]; Vlad Zabrouskov[5]; Michael W. Senko[5]; [1]*Northwestern University, Evanston, IL;* [2]*S.C. Beu Consulting, Austin, TX;* [3]*Thermo Fisher Scientific, Austin, TX;* [4]*Thermo Fisher Scientific, Bremen, Germany;* [5]*Thermo Fisher Scientific, San Jose, CA*

10:30 am - 2:30 pm Wednesday

WEDNESDAY POSTER SESSION
Poster/Exhibit Hall ground level
Lunch concessions are open 11:00 am - 2:00 pm

Odd-number posters present:
10:30 am - 11:30 am PLUS 12:30 - 2:30 pm

Even-number posters present:
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Poster Pick-Me-Up Snacks served at 1:30 pm

2:30 - 4:30 pm Wednesday
METABOLOMICS: UNTARGETED PROFILING
Session Chair: Elizabeth J. Want (Imperial College)
Murphy Ballroom, Bldg B, Level 5

WOA pm 02:30 **Determining the Metabolic Fate of Nitrogen Oxide Species Using Isotopic Tracing and High Resolution Mass Spectrometry**; Steven Mullett[1]; Stacy L. Wendell[2]; *[1]University Of Pittsburgh, Pittsburgh; [2]University of Pittsburgh, Pittsburgh, PA*

WOA pm 02:50 **Single-Cell Metabolomic Analysis of Metastatic and Non-Metastatic Cell Line Pairs Using Mass Spectrometry**; Shelby R Beasley[1]; Mei Sun[1]; Zhibo Yang[1]; *[1]University of Oklahoma, Norman, OK*

WOA pm 03:10 **Enhancing Untargeted Metabolomics with Fast-Scanning Field Asymmetric Waveform Ion Mobility Spectrometry**; James Reynolds[1]; Katarzyna Szykula[1]; Colin Creaser[1]; *[1]Loughborough University, Loughborough, United Kingdom*

WOA pm 03:30 **Development of Advanced Processing Workflow for Untargeted Volatilomics By GC×GC-TOFMS**; Pierre-Hugues Stefanuto[1]; Delphine Zanella[1]; Maurine Fucito[1]; Florence Schleich[2]; Renaud Louis[2]; Jean-François Focant[1]; *[1]Liège University, Liege, Belgium; [2]Liège University Hospital, Liège, Belgium*

WOA pm 03:50 **MetaboPique: A High-Throughput Computational Workflow for Validating, Annotating, and Organizing Small Molecule MS/MS Spectra Derived from Biological Samples**; Tytus D Mak[1]; Concepcion A Remoroza[1]; Meghan C Burke[1]; Kelly H Telu[1]; Stephen E Stein[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

WOA pm 04:10 **A High-Throughput Method for Obtaining Microbial Exometabolomics Data Using a 3D Printed Platform**; Caroline Birer[1]; Rosalie K. Chu[2]; Christopher Anderton[2]; Erik S. Wright[1]; *[1]Department of Biomedical Informatics, University of Pittsburgh, Pittsburgh, PA; [2]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA*

2:30 - 4:30 pm Wednesday
HYDROGEN-DEUTERIUM EXCHANGE MS: INNOVATIONS
Session Chair: Miklos Guttman (University of Washington)
B401-402

WOB pm 02:30 **Advanced Statistical Methods for Analysis of HX-MS Data in Higher-Order Structural Comparability and Similarity Contexts Using Hybrid Significance Criteria**; Tyler S Hageman[1]; David Weis[1]; *[1]University of Kansas, Lawrence, KS*

WOB pm 02:50 **New insights into Differences In Intrinsic HDX Rates at Different pH and Temperature**; Jun Zhang[1]; Devrishi Goswami[2]; zhoangqi Zhang[2]; *[1]Amgen, Inc, Thousand Oaks, CA; [2]Amgen, Inc., Thousand Oaks, CA*

WOB pm 03:10 **Synergistic Structural Information about Stressed Therapeutic Antibodies from Hydrogen Deuterium Exchange and Covalent Labeling Mass Spectrometry**; Catherine Tremblay[1]; Patanachai Limpikirati[1]; Richard W. Vachet[1]; *[1]University of Massachusetts-Amherst, Amherst, MA*

WOB pm 03:30 **Hydrogen-Deuterium Exchange Mass Spectrometry Reveals the Mechanism of Multidrug Resistance in the Efflux Pump AcrB**; Argyris Politis[1]; Zainab Ahdash[1]; Eamonn Reading[1]; Xuan Wang Kan[2]; Elizabeth Grimsey[2]; Laura J. V. Piddock[2]; *[1]King's College London, London, United Kingdom; [2]University of Birmingham, Birmingham, United Kingdom*

WOB pm 03:50 **Rapid Solution-Phase HDX for Small Molecule Identification**; Sandra N Majuta[1]; Chong Li[1]; Kinkini Jayasundara[1]; Ahmad Kiani Karanji[1]; Kushani Attanayake[1]; Nandhini Ranganathan[1]; Peng Li[1]; Stephen Valentine[1]; *[1]West Virginia University.C. Eugene Bennett Department of Chemistry, Morgantown, WV*

WOB pm 04:10 **New Electrochemical Cell for Superior On-line Reduction of Disulfide Bonds in MS Proteomics**; Jean-Pierre Chervet[1]; Pablo Sanz de la Torre[1]; Hendrik Jan Brouwer[1]; Martin Eysberg[2]; *[1]Antec Scientific, Zoeterwoude, Netherlands; [2]Antec Scientific, Boston, MA*

2:30 - 4:30 pm Wednesday
FORENSICS: INNOVATIONS AND APPLICATIONS
Session Chair: Travis M. Falconer (US Food & Drug Administration)
B405-407

WOC pm 02:30 **Rapid and Sensitive Detection of Organic Explosives with PS (Paper Spray) and SAWN Surface Acoustic Wave Nebulization) Ambient Ionization Mass Spectrometry**; Lauren Pintabona[1]; Alina Astefanei[1]; Arian C. Van Asten[1]; Garry L. Corthals[1]; *[1]University of Amsterdam, Amsterdam, Netherlands*

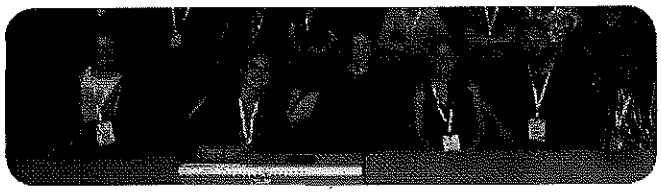
WOC pm 02:50 **Proteomic Profiling of Single Hairs Recovered after an Explosion for Protein-Based Human Identification**; Fanny Chu[1,2]; Katelyn E. Mason[1]; Deon S. Anex[1]; A. Daniel Jones[2]; Bradley Hart[1]; *[1]Lawrence Livermore National Laboratory, Livermore, CA; [2]Michigan State University, East Lansing, MI*

WOC pm 03:10 **Carrion Insect Species Identification From Multi-species Mixtures of Larvae Using Multi-label Classification of DART-HRMS Data for Postmortem Interval Determination**; Rabi A Musah[1]; Samira Beyramysoltan[1]; Justine E. Giffen[1]; Jennifer Y. Rosati[2]; Monica Ventura[1]; *[1]University at Albany-SUNY, Albany, NY; [2]John Jay College of Criminal Justice, New York City, NY*

WOC pm 03:30 **Towards On-Site Drug Evidence Confirmation via Surface-Enhanced Raman Spectroscopy and Paper Spray Ionization Employed on Portable Instrumentation**; William L. Fatigante[1]; Ashley R. Stelmack[1]; Daniel Burr[1]; John Harms[1]; Jeremy D. Driskell[1]; Jun-Hyun Kim[1]; Jamie R Wieland[1]; Christopher Mulligan[2]; *[1]Illinois state university, Normal, IL; [2]Illinois State University, Normal, IL*

WOC pm 03:50 **ASAP Mass Spectrometry for the Real-Time Identification of Psychoactive Drugs Supplied by the Public as Part of a Harm-Reduction Service**; Christopher A Whitmore[1,2]; Guy Jones[2,3]; Fiona Measham[1,2]; Jackie Mosely[1,2]; *[1]Durham University, Durham, United Kingdom; [2]The Loop, Manchester, United Kingdom; [3]Reagent Tests, Cambridge, United Kingdom*

WOC pm 04:10 **Mass Spectrometry-Derived Information Concerning Atypical Findings Critical to Sports Drug Testing: 19-Norandrosterone and AICAR**; Mario Thevis[1]; Frank Huelsemann[1]; Thomas Piper[1]; *[1]German Sport University, Cologne, Germany*



2:30 - 4:30 pm Wednesday
ENDOGENOUS PROTEIN BIOMARKERS IN DRUG DISCOVERY AND DEVELOPMENT: QUANTITATIVE ANALYSIS
Session Chair: Naiyu Zheng (Bristol-Myers Squibb Company)
B302-305

WOD pm 02:30 **A Sensitive LC-HRMS Method for the Quantitation of Dystrophin Protein in Human Muscle Tissue**; Kevork Mekhssian[1]; Hélène Montpetit[1]; Romain Beauvois[1]; Hironori Osaki[2]; Anahita Keyhani[1]; *[1]Altasciences, Laval , QC; [2]NS Pharma, Paramus, NJ*

WOD pm 02:50 **IL2 Receptor α/β/γ Turnover Kinetic Measurement *In vitro* by Serial Immuno Affinity(IA) Capture and Targeted LC/MS Method**; Xiaomeng Shen[1]; Kevin Cook[1]; Yun Ling[1]; Dan A Rock[1]; Brooke Rock[1]; *[1]Amgen, South San Francisco, CA*

WOD pm 03:10 **Interrogation of the Tumor Microenvironment: LCMS-based Quantitation of Target, Drug, and Relevant Biomarkers for Drug Discovery**; Petia Shipkova[1]; Yongxin Zhu[1]; Jacob Zalaznick[1]; Bogdan Sleczka[1]; Matthew Mazur[1]; Karen Parrish[1]; Zheng Yang[1]; Timothy Olah[1]; *[1]Bristol Myers Squibb, Princeton, NJ*

WOD pm 03:30 **Proteomic Analysis Revealed Targeting Crosstalk of Histone H3K27me and H3K27ac as a Therapeutic Strategy for EZH2-Aberrant Solid Tumors**; Minjia Tan[1]; Min Zhang[2]; Xun Huang[2]; Juan Yan[2]; Zhiwei Liu[2]; Linhui Zhai[2]; Jian Ding[2]; Meiyu Geng[2]; *[1]Shanghai Institute of Materia Medica, Shanghai, China; [2]Shanghai Institute of Materia Medica, Shanghai, China*

WOD pm 03:50 **Absolute Quantitation of Cellular Retinol Binding Protein, Type 1 in Cancer-Relevant Cell Lines *via* In-Gel Digestion**; Stephanie Zalesak[1]; Wenjing Li[1]; Jianshi Yu[1]; Maureen Kane[1]; *[1]University of Maryland, Baltimore- School of Pharmacy, Baltimore, MD*

WOD pm 04:10 **Concentration Measurements of 220 Endogenous Proteins in Capillary Blood Using Dried Blood Spots, as Determined by MRM with Peptide Standards**; Azad Eshghi[1]; Adam J. Pistawka[2]; Jun Liu[3]; Michael Chen[4]; Nicholas J. T. Sinclair[1]; Darryl B. Hardie[1]; Monica Elliott[1]; Lei Chen[1]; Rachael Newman[1]; Christoph H. Borchers[1,2,5,6]; *[1]University of Victoria-Genome BC Proteomics Centre, Victoria, BC; [2]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; [3]Department of Pathology and Laboratory Medicine, University of British Columbia, Vancouver, BC; [4]Island Medical Program, Department of Pathology and Laboratory Medicine, University of British Columbia, Vancouver, BC; [5]Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; [6]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC*

2:30 - 4:30 pm Wednesday
CLINICAL ANALYSIS: MS IN THE OPERATING ROOM
Session Chair: Y. Ruben Luo (UCSF)
B308-309

WOE pm 02:30 ***In vivo* and Intraoperative Tissue Analysis and Diagnosis Using the MasSpec Pen**; Jialing Zhang[1]; Marta Sans[1]; Christopher Pirko[2]; Rachel J. DeHoog[1]; Kyana Garza[1]; Clara L. Feider[1]; Mary King[1]; Alena Bensussan[1]; John Q. Lin[1]; Michael Keating[1]; Timothy Hooper[1]; Wendong Yu[2]; Chandandeep Nagi[2]; Sadhna Dhingra[2]; George Van Burren[2]; Stacey Carter[2]; William Fisher[2]; Omar Barakat[2]; Raymon Grogan[2]; Thomas E. Milner[3]; James Suliburk[2]; Livia S. Eberlin[1]; *[1]University of Texas, Department of Chemistry, Austin, TX; [2]Baylor College of Medicine, Houston, TX; [3]University of Texas, Austin, TX*

WOE pm 02:50 ***In vivo* Tissue Classification Using Surgical Robotics and Rapid Evaporative Ionisation Mass Spectrometry – towards the Chemically Aware Surgical Robot**; Eftychios Manoli[1]; Burak Temelkuran[1]; Julia Balog[2]; Steven Pringle[2]; Jagtar Dhanda[3]; Ara Darzi[1]; Neil Tolley[1]; Zoltan Takats[1]; *[1]Imperial College London, London, United Kingdom; [2]Waters Corporation, Wilmslow, United Kingdom; [3]Queen Victoria Hospital, East Grinstead, UK, East Grinstead, United Kingdom*

WOE pm 03:10 **Moving Forward into *in vivo* Intraoperative Diagnostic Using Water-Assisted Laser Desorption/Ionization Mass Spectrometry**; Philippe Saudemont[1]; Nina Ogrinc[1]; Yves-Marie Robin[2]; Benoit Fatou[1,3]; Cristian Focsa[3]; Michael Ziskind[3]; Dominique Tierny[4]; Zoltan Takats[5]; Michel Salzet[1]; Isabelle Fournier[1]; *[1]PRISM Inserm U1192 - University of Lille, Villeneuve D'ascq Cedex, France; [2]Pathology Department, Centre Oscar Lambret, Lille, France; [3]University of Lille, CNRS UMR 8523 PhLAM, Villeneuve d'Ascq, France; [4]OCR, Villeneuve d'Ascq, France; [5]Imperial College London, Department of Surgery and Cancer, United Kingdom*

WOE pm 03:30 **Infrared Laser Based Real-Time, *in vivo* Tissue Identification in Veterinary Surgery Using Laser-Assisted Rapid Evaporative Ionization Mass Spectrometry**; Viktoria Varga[1]; Steven D Pringle[2]; Gabriel Stefan Horkovitcs-Kovats[3]; Julia Balog[3]; *[1]Waters Research Center Kft., Budapest, Hungary; [2]Waters Corporation, Wilmslow, United Kingdom; [3]Waters Research Center, Budapest, Hungary*

WOE pm 03:50 **Implementation of Ambient MS-Based Tissue Profiling for Assistance on Neurosurgery Operations of Brain Cancer**; Igor Popov[1]; Anatoly Sorokin[1,2]; Vsevolod Shurkhay[3]; Vasiliy Eliferov[1]; Evgeny Zhvansky[1]; Stanislav Pekov[1,4]; Alexander Potapov[3]; Eugene (evgeny) Nikolaev[5]; *[1]Moscow Institute of Physics and Technology (State University), Dolgoprudny, Russia; [2]Institute of Cell Biophysics RAS, Pushchino, Russia; [3]N. N. Burdenko Scientific Research Neurosurgery Institute, Moscow, Russia; [4]Institute for Energy Problems of Chemical Physics RAS, Moscow, Russia; [5]Skolkovo institute of science and technology, Moscow Region, Russian Federation*

WOE pm 04:10 **Qualitative Classification of Tissue Amyloidosis and Subtyping by Mass Spectrometry**; Srinivas V.s Chakravartula[1]; Adolfo Firpo Betancourt[2]; Damodara Rao Mendu[3]; Tin Htwe Thin[2]; Salem Fadi[3]; Michael Donovan[2]; Carlos Cordon Cardo[2]; *[1]Mount Sinai Hospital, New York City, New York; [2]Icahn School of Medicine at Mount Sinai, New York, NY; [3]Mount Sinai Hospital, New York City, NY*

2:30 - 4:30 pm Wednesday
ION MOBILITY: SMALL MOLECULES, PHARMACEUTICALS, AND DMPK
Session Chair: Erin Baker (North Carolina State University)
B312-314

WOF pm 02:30 **Clinical Metabolomics Study Uncovers the Outcome of Radiation Therapy in Cancer Patients**; Nicholas B. Vera[1,2]; Evan Pannkuk[3];

Evagelia C Laiakis[3]; Albert J Fornace[3]; Stephen L. Coy[2]; Michelle Clasquin[1]; Paul Vouros[2]; *[1]Pfizer, Internal Medicine Research Unit, Cambridge, MA, 02139; [2]Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA 02115; [3]Georgetown University, Washington, DC*

WOF pm 02:50 **Characterization of Gas-Phase Structures of Drug Metabolites Using Ion Mobility-Mass Spectrometry**; Dylan H. Ross[1]; Ryan P. Seguin[1]; Libin Xu[1]; *[1]University of Washington, Seattle, WA*

WOF pm 03:10 **DMS Separation, IR Identification, and Quantification of Amino Acids and Related Compounds in Plasma Samples**; Francis Berthias[1]; Yali Wang[1]; Eskander Alhajji[1]; Jean-François Benoist[2]; Philippe Maitre[3]; *[1]Université Paris-Sud, Orsay, France; [2]Hôpital Robert Debré, Paris, France; [3]Université Paris Sud, Orsay, France*

WOF pm 03:30 **Rapid Detection of Fentanyl Analogs Using GC-APCI-TIMS-TOF MS**; Elisa N Shoff[1,2]; Cesar E Ramirez[1]; Francisco A. Fernandez-Lima[1]; *[1]Department of Chemistry and Biochemistry, Florida International University, Miami, FL; [2]Miami-Dade Medical Examiner Department, Miami, FL*

WOF pm 03:50 **Development of Ion Mobility-Mass Spectrometry Methods and Collision Cross Section Database for Improved Identification of Microbiome-Derived Metabolites**; Matthew Glover[1]; Omari Jones-Nelson[1]; Taylor Cohen[1]; Wen Yu[1]; Paul Warrener[1]; Bret Sellman[1]; Sonja Hess[1]; *[1]MedImmune, Gaithersburg, MD*

WOF pm 04:10 **Imaging Mass Spectrometry Including Ion Mobility Separation Sheds Light on Bacterial Responses to Different Cultivation Conditions**; Francesca Brescia[1,2]; Samuele Zoratto[3]; Gerardo Puopolo[2]; Ilaria Pertot[2]; Martina Marchetti-deschmann[3]; *[1]Department of Sustainable Ecosystems & Bioresources, Research and Innovation Centre, Fondazione Edmund Mach, San Michele all'Adige, Italy; [2]Department of Agricultural, Food, Environmental and Animal Sciences, University of Udine, Udine, Italy; [3]Institute of Chemical Technologies and Analytics, TU Wien, Vienna, Austria*

2:30 - 4:30 pm Wednesday
INSTRUMENTATION: AMBIENT IONIZATION AND APPLICATIONS
Session Chair: G. Asher Newsome (Smithsonian Institution)
Auditorium, Bldg A

WOG pm 02:30 **First implementation of Rapid Evaporative Ionisation Mass Spectrometry (REIMS) for the At-Line Screening of Boar Carcasses in the Slaughter House**; Lieselot Y Hemeryck[1]; Sara L Stead[2]; Anneleen Decloedt[1]; Steve Huysman[1]; Julia balog[3]; Margot DeSpiegeleer[1]; Steven D Pringle[2]; aurelien boland[4]; Lynn Vanhaecke[1]; *[1]Ghent University, Ghent, Belgium; [2]Waters Corporation, Wilmslow, United Kingdom; [3]Waters Research Centre, Budapest, Hungary; [4]Waters Benelux, Brussels, Belgium*

WOG pm 02:50 **A Single-Cell Look at Biological Nitrogen Fixation: Rapid Determination of Metabolite Formulas from Isotopic Fine Structures in Heterogeneous Cell Populations**; Laith Z Samarah[1]; Rikkita Khattar[1]; Tina H Tran[1]; Sylwia A Stopka[1]; Dusan Velickovic[2]; Christopher R Anderton[2]; Jared B. Shaw[2]; Nikola Tolic[2]; David W Koppenaal[2]; Ljiljana Pasa-Tolic[2]; Beverly J Agtuca[3]; Gary Stacey[3]; Akos Vertes[1]; *[1]The George Washington University, Washington, DC; [2]Pacific Northwest National Laboratory, Richland, WA; [3]University of Missouri, Columbia, MO*

WOG pm 03:10 **MicroArray Droplet Ionization for Spatially Controlled Imaging of Lipids and Metabolites in Biological Samples**; Marta Sans[1]; Anna Krieger[1]; Bryan Wygant[1]; Kyana Garza[1]; C. Buddie Mullins[1,2]; Livia S. Eberlin[1]; *[1]University of Texas, Austin, TX; [2]McKetta Department of Chemical Engineering, The University of Texas, Austin, TX*

WOG pm 03:30 **Charge Production by Sublimation of Organic Compounds in Matrix Assisted Ionization**; Bijay Banstola[1]; Kermit K. Murray[1]; *[1]Louisiana State University, Baton Rouge, LA*

WOG pm 03:50 **Understanding the Implications of Confined DART-MS: Considerations and Strategies for Optimization**; Edward Sisco[1]; Thomas P. Forbes[2]; Matthew Staymates[2]; *[1]National Institute of Standards and Technology, Gaitherburg, MD; [2]National Institute of Standards and Technology, Gaithersburg, MD*

WOG pm 04:10 **Ion Focusing and Transport in Air Using Conductive 3D-Printed Electrodes**; Kiran Iyer[1]; Brett M Marsh[1]; Grace Olivia Capek[1]; Shane Tichy[2]; Graham R. Cooks[1]; *[1]Purdue University, West Lafayette, IN; [2]Agilent Laboratories, Santa Clara, CA*

2:30 - 4:30 pm Wednesday
FUNDAMENTALS: DDA AND DIA LC-MS
Session Chair: Stefan Tenzer (University Medical Center Mainz)
A411-412

WOH pm 02:30 **diaPASEF: Toward the Ideal Mass Analyzer with Data-Independent Acquisition and Parallel Accumulation – Serial Fragmentation**; Florian Meier[1]; Andreas-David Brunner[1]; Max Frank[2]; Annie Ha[2]; Eugenia Voytik[1]; Stephanie Kaspar-Schönefeld[3]; Markus Lubeck[3]; Heiner Koch[3]; Scarlet Koch[3]; Oliver Raether[3]; Ben C Collins[4]; Ruedi Aebersold[4,5]; Hannes Röst[2]; Matthias Mann[1,6]; *[1]Max-Planck-Institute of Biochemistry, Martinsried, Germany; [2]Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON; [3]Bruker Daltonik GmbH, Bremen, Germany; [4]ETH Zurich, Zurich, Switzerland; [5]University of Zurich, Zurich, Switzerland; [6]University of Copenhagen, Copenhagen, Denmark*

WOH pm 02:50 **Combining Drift Tube Ion Mobility and Quadrupole Selectivities for Data Independent Workflows for Metabolomics**; Tim Causon[1]; Max Feuerstein[1]; Ruwan T. Kurulugama[2]; George Stafford[2]; John C. Fjeldsted[2]; Stephan Hann[1]; *[1]Institute of Analytical Chemistry, Department of Chemistry, University of Natural Resources and Life Sciences (BOKU), Vienna, Austria; [2]Agilent Technologies, Inc., Santa Clara, CA*

WOH pm 03:10 **Improving Quantification Using MS1 and MS2 Information in Data Independent Acquisition**; Roland Bruderer[1]; Ting Huang[2]; Jan Muntel[1]; Oliver M. Bernhardt[1]; Olga Vitek[2]; Lukas Reiter[1]; *[1]Biognosys, Schlieren, Switzerland; [2]Khoury College of Computer and Information Sciences, Boston, MA*

WOH pm 03:30 **TKO-iQC: A Platform for Tracking Instrument Performance and Evaluating Interference in Isobaric Tag-based Workflows**; Joao A Paulo[1]; Jose Navarrete-Perea[1]; Steven P Gygi[1]; *[1]Harvard Medical School, Boston, MA*

WOH pm 03:50 **Using an External Reference Material to Harmonize and Calibrate Quantitative Mass Spectrometry Data at Scale**; Lindsay Pino[1]; Brian C Searle[2]; Han-Yin Yang[1]; Andrew N Hoofnagle[3]; William Stafford Noble[1]; Michael J MacCoss[1]; *[1]University of Washington, Genome Sciences, Seattle, WA; [2]Institute for Systems Biology, Seattle, WA; [3]University of Washington, Seattle, WA*



WOH pm 04:10 **Defying Gravity in Orbitrap Mass Spectrometry**; Jan-Peter Hauschild[1]; Amelia Peterson[1]; Erik Couzijn[1]; Eduard Denisov[1]; Denis Chernyshev[1]; Christian Hock[1]; Hamish Stewart[1]; Ralf Hartmer[1]; Christian Thoeing[1]; Oliver Lange[1]; Mathias Mueller[1]; Arne Kreutzmann[1]; Wilko Balschun[1]; Aivaras Venckus[1]; Alexander Kholomeev[1]; Gregor Quiring[1]; Frank Czemper[1]; Tabiwang N. Arrey[1]; Kerstin Strupat[1]; Julia Kraegenbring[1]; Markus Kellmann[1]; Alexander Harder[1]; Alexander Makarov[1]; *[1]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

4:45-5:30 pm Wednesday
ASMS MEETING
Richard A. Yost (University of Florida), presiding
Enjoy a beverage and hear the latest ASMS news.
B302-305

5:45 - 7:00 PM WEDNESDAY WORKSHOPS

There will be light refreshments in Building A foyers. All workshops are in Building A.

01 MS-Based Interactomics: Computational Resources and Tools for Studying the Physical Interactome
(Bioinformatics MS Interest Group)
Presiding: Isabell Bludau, William Noble
A402-403

The large variety of molecular functions in living systems are frequently not performed by single molecules, but are a result of the interplay between different molecular entities. Proteins, metabolites, lipids, RNA and DNA molecules interact among themselves and with each other to give rise to a large variety of functional modules inside the cell. Studying the quantity, subunit composition and topology of these modules and their dynamic change upon perturbations is therefore of fundamental interest for biology. In this workshop, we aim to introduce and discuss various strategies to analyze the physical interactome of biological molecules. We will specifically focus on available resources and software tools for (a) the in silico prediction of interactions, (b) the computational analysis of large-scale interactomics datasets (including AP-MS, cross-linking MS, protein correlation profiling, LiP-MS, etc.) and (c) the integration of data generated by multiple orthogonal strategies. We will invite leading experts in the field to present an overview of available databases and software tools as well as to provide general guidelines on their usability for different applications. Finally, we will discuss recent developments and future perspectives in the area of MS-based interactomics.

02 IMS: When Chromatography Just Won't Do
(Ion Mobility MS Interest Group)
Presiding: Brian Clowers, Jakub Ujma, Ian Webb
A404-405

Fundamental measurements of gas-phase ion properties serve as the foundation describing ion mobility (IM); this property is often exploited for analytical benefits. With historical names such as Plasma Chromatography and Gaseous Electrophoresis, ion mobility techniques often have logical analogues to more traditional chromatographic techniques. Until recently, the major differentiator between IM separations and contemporary chromatographic techniques was the speed of analysis.

Advances in ion confinement and manipulation (e.g. ion funnels, T-wave, and SLIM technologies) allowed increases in the separation path lengths, thus significant enhancements in resolving power (Rp) have been achieved; often at a cost of increased separation time scales. Improvements in Rp can also be achieved by increasing the strength of the applied electric field. This, in principle offers increased Rp and reduced separation time scale, but several practicalities have to be considered. As the separating power of ion mobility techniques increases, the additional pressures are placed on the mass spectrometry systems used for detection. More specifically, as peak widths narrow in the temporal domain, minimizing peak broadening in the IM-MS transfer region (equivalent to extra-column broadening in chromatography) becomes paramount as well as compatibility of MS analyser/detector with the high fidelity ion mobility distributions.

To provide the community with a contemporary view of ion mobility-mass spectrometry techniques this forum will highlight the emergent, fast approaches to enhance separation selectivity of gas-phase ions. This workshop will cover methods hyphenated with IM, in particular those benefiting from the speed of IM separation. Finally, this workshop aims to promote discussion about the role of ion mobility techniques in tandem with chromatographic techniques and in some cases serve as a rapid replacement for front end separations prior to mass analysis.

03 Clinical Applications: Standardization and Harmonization Efforts
(Clinical Chemistry Interest Group)
Presiding: Candice Ulmer, Donald Chace
A406-407

With the advent of novel mass spectrometric reference measurement procedures and improved clinical analyzers for clinical diagnostics, standardized results have become a necessity in the clinical setting to ensure accuracy/reliability in laboratory measurements, consistent disease diagnosis, and appropriate treatment for patients. Standardization ensures that laboratory testing is accurate, reliable, and precise across methods and over time. In addition, standardization is important in the clinical setting as many clinical/public health decisions are made and evidence-based patient guidelines written using laboratory measurements. Comparable measurements are needed between multiple assays, including those performed on clinical analyzers and mass spectrometers to allow for the generation of analyte-specific reference values. As a means to harmonize immunoassays and mass spectrometric procedures, reference materials and international standards are needed for method calibration purposes and conversion values. This workshop will [1] highlight the need for harmonized results, [2] introduce ongoing standardization efforts within clinical chemistry, and [3] discuss opportunities to create and engage in commutability studies, certification programs, and clinical-based interlaboratory studies.

04 Exposomics Workshop
(Exposomics Interest Group)
Presiding: Jarod Grossman, Silvia Balbo, Benedikt Warth
A408

This workshop will have a panel consisting of thought leaders in different scientific fields of the exposome space. They will discuss their work and challenges they have overcome and encountered in their research.

Global interest in the exposome is growing and this expansion can be seen in the increased number of exposome publications in peer reviewed journals since 2010. There are many funded research endeavors designed to 'explore the exposome.' In the EU, HEALS,

There will be light refreshments in Building A foyers. All workshops are in Building A.

HELIX and EXPoSOMICS are all underway. PI's represent Imperial College, London, Aristotle University of Thessaloniki and CREAL in Barcelona. The Phenome Center has been established at Imperial College, London. In the US, NIEHS has funded HERCULES at Emory University and US EPA and CDC both define the exposome as a critical entity required to better understand the non-genetic contribution to chronic disease. Moreover, major US and Canadian Universities including Harvard, University of Pennsylvania, Stanford, University of Alberta and those mentioned above are engaged in exposome research. In Japan, NIES is conducting a prospective mother / child cohort, with more than 300,000 participants, to measure the exposome and in China, several University's are moving away from measuring pollutants in air and water, and into the exposome paradigm.

05 MS-Based Process Analytical Technology (PAT): Testing & Control of CQAs
(Pharmaceuticals Interest Group)
Presiding: Andrew Dawdy, Richard Rogers
A410

One major goal of biotherapeutic process development (PD) is to produce the same high quality product in every experiment regardless of scale. To achieve this goal, PD scientists need to employ process analytical technologies (PAT) that can provide data on the upstream process (e.g. temperature, pH, glucose, amino acids, cell viability, and metabolites), downstream process (e.g. process-related impurities and host-cell impurities) and product quality attributes of the final product (e.g. charge isoforms, aggregates, and glycoforms). Mass spectrometry is an extremely valuable tool for characterizing bulk drug substance to identify critical quality attributes that affect the safety and efficacy of the product. However, MS-based PAT may also be used to characterize in-process molecules and study other upstream and downstream parameters that dictate the attributes of the final product. This workshop will be an interactive discussion amongst a panel of experts and the workshop attendees on the current state of mass spectrometry-based PATs and how they are improving PD. Topics may include application of MS for real-time (on-line / at-line) analysis of in-process materials, quality by design (QbD), continuous biomanufacturing, automated sample handling / preparation, automated data processing (e.g. intact deconvolution), novel technologies for MS-based charge isoform characterization, application of proteomics or metabolomics to support process development, and others. Please join us to ask questions, share your knowledge and experience, and discuss the future of MS-based PAT for the development of biotherapeutics.

06 Endogenous Biomarkers: Measurement to Predict in vivo Drug-Drug Interactions
(DMPK Interest Group)
Presiding: Jonathan Josephs, Brian Rago, Aaron Teitelbaum
A307

Current in vitro models at assessing drug-drug interaction (DDI) liability of a new chemical entity (NCE), though the gold standard in drug discovery, struggle with a high false-positive rate (~30%). The ability to interrogate a validated transporter biomarker, in early clinical studies, such as first-in-human (FIH) studies, would help assess DDI liability, complement the existing agency DDI risk assessment approaches, help confirm or dispute in vitro data and potentially reduce the number of dedicated DDI clinical evaluations. This could result in earlier discharging of DDI risk and lead to significant resource and time savings.

Endogenous biomarkers of CYP and transporter activity have emerged recently as a growing area of interest for biomarker research and may provide insights into the potential for clinical DDIs without the need to conduct a specific clinical trail with a probe substrate. In addition to the traditional CYP enzymes considered. Transporters include OATP1B1/1B3, OCT1, OAT2, NTCP, OCT2, MATE1 and MATE2K. Recently, publications have explored coproporphyrin isomers (CP-I and CP-III), bile acids (BAs), and N1-methylnicotinamide as potential OATP1B1/3 and renal OCT2 transporter biomarkers, respectively. Additionally, thiamine and 6β-hydroxycortisol have been proposed as possible endogenous probes for hepatic OCT1 and renal OAT3, respectively. Creatinine has been proposed as a biomarker for OCT2, MATE1 and MATE2K inhibition.

While using traditional triple quadrupole based assays for biomarker quantitation has been well demonstrated for a number of these biomarkers. Using UHPLC-HRMS to interrogate potential biomarkers has several advantages: targeted quantitation, multiplexing of biomarkers, and also post-acquisition data mining of novel biomarkers.

07 The NIH and NSF Review and Funding Process
Presiding: Salvatore Sechi, Kelsey Cook, Douglas Sheeley
A309

Many ASMS members and conference participants are supported by the National Institutes of Health or the National Science Foundation. During this workshop the general funding and review process of grant applications/proposals will be presented. Issues like identifying the best contacts, writing an effective application/proposal, and responding to the reviewers' criticisms will be discussed. Speakers will explore these issues from the perspectives of the applicant, reviewer, and administrator, with some emphasis on new investigators and training opportunities. Tips on grant writing and insights into the review process will be presented. Substantial time will be allotted for discussion and questions. NIH and NSF staff will also be available for individual discussions with investigators during scheduled "Office Hours" in the poster exhibit hall.

08 Why You Should Submit Your Best Manuscripts to *JASMS*
Presiding: Joe Loo, *JASMS* Editor-in-Chief
A311

The *Journal of the American Society for Mass Spectrometry (JASMS)* was started in 1990, and it remains a premier science journal that covers all aspects of mass spectrometry, including fundamental subjects (e.g., properties of gas-phase ions, instrumentation design, etc) and applications of mass spectrometry in all fields (including chemistry, biology, physics, geology, environmental science, and life sciences). But the scientific publishing industry has undergone dramatic changes since 1990, and journals must keep pace with these changes in order to remain competitive. The Workshop will discuss the current "nuts and bolts" of the operation of JASMS, how manuscripts are handled, how the journal can grow to best serve the needs of the mass spectrometry scientific community and the members of ASMS, and why all members should consider submitting their best work to the Society's journal. Members from the JASMS Editorial Staff and the ASMS Publications Committee will spur lively discussions.

09 Metaproteomics for the Masses: Solutions, Opportunities and Challenges
Presiding: Pratik Jagtap, Timothy Griffin, Robert Hettich
A312

Metaproteomics, which characterizes the protein complement of a microbiome, enables researchers to understand the network and functional roles of the expressed microbial proteins in an ecosystem, thereby opening new avenues to characterize a variety of eukaryotic (human, plant) and environmental (soil, ocean) systems. As a complement to nucleic-acid based metagenomics (which provide detailed taxonomic information about microbial composition), metaproteomics research provides information about the metabolic activities and mechanism of microbial interactions with the host or environment. However, as compared to single-organism proteomics, mass spectrometry-based metaproteomics research poses additional challenges in data acquisition, database searching, and information extraction from these very complex peptide mixtures. Moreover, advanced bioinformatics approaches are needed to properly assign peptides to appropriate proteins and functional groups, as well as handle quantitative and multi-replicate analyses.



There will be light refreshments in Building A foyers. All workshops are in Building A.

Metaproteomics research experts will discuss the current status of metaproteomics research, and highlight solutions and opportunities in the emerging field. In particular, advanced data acquisition strategies and database searching methods for peptide matching and metaprotein inference will be discussed. Experts will also participate in an informal discussion on multi-omic studies (metagenomics, metatranscriptomics, metaproteomics, and metabolomics) and quantitative and statistical analysis of multi-replicate samples.

10 Bridging the Gap between Computational Biology and Biology: Matchmaking Session
Presiding: Ewy Mathe, Corey Broeckling
A313

Nowadays, science is conducted collaboratively and most often requires experts in bench (e.g. chemistry, biology) and computational sciences. The goal of this workshop is to promote conversations between computational biology, chemistry, and biology experts and to help bridge the communication gap between the fields. While bench scientists seek help with analysis of their data, computational biologists are hungry for data to test out their solutions to data analysis problems. The aim of this workshop is thus discuss methods to bridge the language and culture gap between computational biology and biology. A secondary aim is to help researchers find each other in this large conference setting.

The session will be split into three parts: 1) brief introduction; 2) all participants share their work in 3-5 minutes; 2) informal, small group discussions (led by moderators), where tool developers/analysis experts interact with bench scientists/novice researchers to identify common interests and foster future conversations/collaborations. Topics will include broad aspects of metabolomics analysis, from data preprocessing, to statistical analyses and data interpretation.

11 Ambient Ionization: Where We Stand Now and Go from Here
Presiding: Bindesh Shrestha, Sylwia Stopka
A314

After the introduction of desorption electrospray ionization (DESI) in the mid-2000s, dozens of new ambient mass spectrometry ionization source have been introduced. These ambient ionization tools are capable of direct analysis of samples in real time, require minimal sample perturbation, and analysis is performed under native conditions. The workshop will begin with a brief introduction that addresses the current state of ambient ionization techniques, followed by brief short presentations on variations of ambient ionization methods. These brief presentations will have a maximum of four slides, consisting of introduction (slide 1), a unique or high impact application (slide 2), limitations of the technique (slide 3), and future direction and discussions (slide 4). The brief presentations will be followed by an open discussion forum focused on current challenges related to ambient ionization and its future direction. The workshop aims to encourage the participation and presentations of new investigators, postdocs, and graduate students with a balanced perspective from academia, national lab, and industry. One of the goals of the workshop will be to gather scientists interested in ambient ionization technology and start the discussion towards forming an ambient ionization interest group to address these new scientific challenges.

12 The Proteomics Standards Initiative and ProteomeXchange: Supporting Open Data Practises in Proteomics
Presiding: Juan Antonio Vizcaino, Eric Deustch, Nuno Bandeira
A315

The Proteomics Standards Initiative (PSI, http://www.psidev.info) and ProteomeXchange (http://www.proteomexchange.org) are two highly collaborative projects that are open to the contribution and ideas from everyone in the community. Since 2002, the mission of the PSI is the development and promotion of open data standards and the related software in the proteomics field. Additionally, the PSI is increasingly involved in the development of data standards for metabolomics. In a parallel effort, since 2012, the ProteomeXchange Consortium is standardising the submission and dissemination of public proteomics data between the main proteomics data repositories, currently including the resources PRIDE, PeptideAtlas, MassIVE, jPOST, iProx and Panorama Public.

We will briefly showcase our most successful projects and highlight some of our ongoing activities, fostering discussion among participants about what future directions in both initiatives would most benefit the community. Please attend if you want your voice to be heard!

13 Fundamentals: Structural Elucidation of Proteins (Fundamentals Interest Group)
Presiding: Christian Bleiholder, Alexandre Shvartsburg
A316

Elucidation of molecular structure has been a key goal of mass spectrometry since its origins, normally achieved using tandem mass spectrometry (MS/MS) via collision-induced dissociation (CID). With the emergence of biological MS, that direction has extended to proteins and their assemblies. The major new challenges faced by structural MS in this context have been (1) critical higher-level structure (beyond primary) and connectivity of post-translational modifications not amenable to standard MS/MS approaches and (2) for primary structure, the molecular size and complexity resulting in numerous competing fragmentation pathways and thus spectral congestion. These issues have motivated the invention of novel structural tools - both expanding the MS/MS capability (via new activation and fragmentation techniques resulting in more informative products) and complementary methods based on ion mobility for overall morphology characterization and/or spectroscopy for more targeted local probes. The central path forward appears to be combining orthogonal approaches in hyphenated instrumentation to provide specific and redundant independent constraints, and developing and validating the structure-property computational models to extract the utmost information from available rich experimental data.

We will discuss the latest instrumental and methodological advances in the area across the leading approaches, highlighting their limitations that one must appreciate tor successful outcomes.

Topics and tentative speakers:

- Primary structure (bottom-up and top-down): Alan Marshall
- Primary structure (top-down and complex-top-down): Neil Kelleher
- Native MS (activation methods and H/D exchange)
- Theory and ion mobility: David Russell
- Spectroscopy: Jennifer Brodbelt

14 Education: Teaching MS at the Undergraduate Level (Undergraduate Research in MS Interest Group)
Presiding: Chrisi Hughey, Jay Forsythe
A303

This workshop will provide an overview of resources available to current and/or future instructors who teach mass spectrometry at the undergraduate level. Attendees are encouraged to bring and share mass spectrometry-related materials that they have developed for lecture and/or the laboratory. We will also discuss the successes and challenges of teaching mass spectrometry at the undergraduate level. The goal of the workshop is to build a community of instructors and an online repository of instructional resources through ASMS and/or the Analytical Sciences Digital Library (ASDL). If you have materials you would like to share, please email hugheyca@jmu.edu.

15 New Ion Manipulations Prior to FT-MS (FTMS Interest Group)
Presiding: Matthew Renfrow, Lissa Anderson,
A302

The efficiency of ion trapping and transferring prior to FT-MS detection has continued to improve and the sophistication of ion manipulations and separations prior to high resolution detection continue to increase.



5:45 - 7:00 PM WEDNESDAY WORKSHOPS AND THURSDAY MORNING ORAL SESSIONS

There will be light refreshments in Building A foyers. All workshops are in Building A.

This year's FT-MS workshop will focus on new ion manipulations prior to FT-MS and what new type of FT-MS-based analysis and experimentation these developments will allow. This includes, but is not limited to, proton transfer reactions, parallel ion parking, ion mobility separations, and other novel additions to the FT-MS field. Experts from academia and industry will be available to help answer questions. The goal is to give users a preview of what future directions ions be moving as the field of FT-MS continues to expand.

16 Cannabis and Hemp Testing Requirements: How to Leverage with Mass Spectrometry
Presiding: Marc Engel, Markus Roggen, Kevin Smith
A301

This workshop will discuss the challenges associated with testing cannabis and cannabis concentrate (edibles, extracts, tincture etc) samples; in addition, Mass Spectrometry techniques suitable for quantifying cannabis will be presented in detail to emphasize their merit for each chemistry group (pesticides, mycotoxins, heavy metals, terpenes etc). Industry thought leaders from the US and Canada will present their latest findings on sample preparation, instrumentation configuration, and data processing specifics to quantitate cannabis and cannabis extract samples in a high throughput environment. Group discussions will also include identifying mass spectrometry topics and research opportunities within cannabis & hemp science that can support this rapidly expanding scientific landscape.

17 Getting Started with R for Mass Spectrometry Data Analysis
Presiding: Ryan Benz, Jeff Jones
A305

This workshop, targeted at beginner and aspiring R users, will introduce the R programming language and the ways it can be used for mass spectrometry data analysis (and data analysis in general). The workshop will start with a gentle introduction to R and the basics of using RStudio, followed by essential data manipulation and analysis strategies using base R and tidyverse packages. Finally, analysis examples utilizing various mass spectrometry specific R packages will be presented. The goal of this workshop is to help new R users get over some of the initial roadblocks beginners often face and to kickstart their efforts toward learning how to use R effectively for data analysis tasks. Bring your laptop to follow along with the examples. Preparatory material for the workshop will be provided at:
https://github.com/ZenBrayn/asms-2019-r-workshop

18. Career and Collaboration Opportunities in China
Presiding: Jun Qu, Andy Tao
A304

Recent economic development in China has created numerous job opportunities for postdoctoral fellows and graduate students with training in mass spectrometry. The overall objective of this workshop is to provide information to those individuals with interest in seeking academic or industrial positions in China. We plan to invite 6-7 mass spectrometrists from academia, pharmaceutical companies, and instrument vendors in China as panel members for this workshop. These individuals will share with the participating graduate students and postdocs about their experiences and perspectives in finding jobs, establishing an independent research program in universities, opportunities available to mass spectrometrists, and developing international collaborations in China. We believe that the workshop will benefit young and next-generation scientists in mass spectrometry by providing a unique perspective of job and research opportunities in China and assisting with their career development. The workshop will be mixed with panelist presentations and Q/A session with the participating students and postdocs.

THURSDAY MORNING ORAL SESSIONS

From 7:00 am Thursday
CORPORATE BREAKFAST SEMINARS
CONVENTION CENTER ONLY
See page 16 for detailed schedule. Reservation or RSVP required.

8:30 - 10:30 am Thursday
INFORMATICS: METABOLOMICS
Session Chair: Caroline Johnson (Yale School of Public Health)
Murphy Ballroom, Bldg B, Level 5

ThOA am 08:30 **OpenSWATH Enables Automated Data Processing for Data-Independent Acquisition in Metabolomics**; Oliver Alka[1]; Michael Witting[2,3]; Karin Kleigrewe[4]; Oliver Kohlbacher[1,5,6,7]; Hannes L. Röst[8]; *[1]Applied Bioinformatics, Department of Computer Science, University of Tübingen, Tübingen, Germany; [2]Helmholtz Zentrum München, Research Unit Analytical BioGeoChemistry (BCG), Neuherberg, Germany; [3]School of Life Sciences Weihenstephan, Technical University of Munich, Freising, Germany; [4]Bavarian Center for Biomolecular Mass Spectrometry (BayBioMS), Technical University of Munich, Freising, Afghanistan; [5]Quantitative Biology Center, University of Tübingen, Tübingen, Germany; [6]Biomolecular Interactions, Max Planck Institute for Developmental Biology, Tübingen, Germany; [7]Institute for Translational Bioinformatics, University Hospital Tübingen, Tübingen, Germany; [8]Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON*

ThOA am 08:50 **Development of a Unified Collision Cross Section Compendium for Compound Annotation and Chemical Class Prediction**; Jaqueline A. Picache[1]; Bailey S. Rose[1]; Andrzej Balinski[1]; Katrina L. Leaptrot[1]; Stacy D. Sherrod[1]; Jody C. May[1]; John A. McLean[1]; *[1]Vanderbilt University, Nashville, TN*

ThOA am 09:10 **Lipid Annotator: A Rapid, Accurate, and User-Friendly Software for Comprehensive LC-HRMS/MS Lipidomics**; Jeremy Koelmel[1]; Xiangdong Li[2]; Sarah Stow[2]; Mark Sartain[2]; Adithya Murali[2]; Robin H.J Kemperman[1]; Richard A Yost[1]; Timothy J. Garrett[1]; Norton Kitagawa[1]; *[1]University of Florida, Gainesville, FL; [2]Agilent Technologies, Santa Clara, CA*

ThOA am 09:30 **Extracting Molecular Knowledge from METASPACE, a Community Knowledge Base of Spatial Metabolomes**; Theodore Alexandrov[1,2]; Katja Ovchinnikova[1]; Andrew Palmer[1]; Vitaly Kovalev[1]; Lachlan Stuart[1]; Artem Tarasov[1]; Renat Nigmetzianov[1]; Dominik Fay[1]; *[1]Structural and Computational Biology Unit, European Molecular Biology Laboratory, Heidelberg, Germany; [2]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA*

ThOA am 09:50 **Improved Interpretation of Metabolomics Data Integrated with other Omics Data: Linear Modeling and Comprehensive Pathway Analysis Approaches**; Jalal K. Siddiqui[1]; Shunchao Wang[1]; Rohith Vanam[1]; Andrew Patt[1]; Joseph McElroy[1]; Ewy Mathe[2]; *[1]The Ohio State University, Columbus, OH; [2]Ohio State University Medical Center, Columbus, OH*

ThOA am 10:10 **Improving Annotation Propagation on Molecular Networks through Random Walks: Introducing ChemWalker**; Ricardo Silva[1,2]; Pieter Dorrestein[3]; *[1]University of California, San Diego, CA; [2]NPPNS, Department of Physics and Chemistry, School of Pharmaceutical Sciences of Ribeirão Preto, University of São Paulo, Ribeirão Preto, Brazil; [3]University of California San Diego, La Jolla, CA*

8:30 - 10:30 am Thursday
FUNDAMENTALS: ION SPECTROSCOPY
Session Chair: Mary T. Rodgers (Wayne State University)
B401-402

ThOB am 08:30 **Integration of High-Resolution Mass Spectrometry with Cryogenic Ion Vibrational Spectroscopy**; Evan H Perez[1]; Fabian Menges[1]; Sean Edington[1]; Chinh Duong[1]; Nan Yang[1]; Mark Johnson[1]; *[1]Yale University, New Haven, CT*

ThOB am 08:50 **Comparing Ultrahigh-Resolution Ion-Mobility Spectrometry and IR-IR Double Resonance Spectroscopy for Isomer-Resolved Spectra of Oligosaccharides**; Robert Pellegrinelli[1]; Stephan Warnke[1]; Ahmed Ben faleh[1]; Yalovenko Natalia[1]; Thomas R. Rizzo[1]; *[1]Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*

ThOB am 09:10 **Two-Color IRMPD Applied on Cryogenically Cooled Peptides: Comparisons to Traditional IRMPD and IR-UV Double Resonance Techniques**; Christopher P. Harrilal[1]; Timothy S. Zwier[1]; Scott A. Mcluckey[1]; *[1]Purdue University, West Lafayette, IN*

ThOB am 09:30 **Circular Dichroism Mass Spectrometry of Biomolecular Ions**; Steven Daly[1]; Frédéric Rosu[2]; Valérie Gabelica[1]; *[1]Université de Bordeaux, INSERM U1212, CNRS UMR 5320, IECB, Pessac, France; [2]Université de Bordeaux, CNRS UMS3033, IECB, Pessac, France*

ThOB am 09:50 **Gas-Phase Fluorescence from Trapped Biomolecular Ions: Instrumentation and Photophysical Studies**; Prince Tiwari[1]; Jonas B Metternich[1]; Martin F Czar[1]; Renato Zenobi[1]; *[1]ETH Zurich, Switzerland*

ThOB am 10:10 **Structures of Hydrogen-Rich DNA Tetranucleotide Cation Radicals toward Achieving Atomic-Resolution by UV/Vis Action Spectroscopy**; Shu R. Huang[1]; Yue Liu[1]; Yang Liu[1]; Frantisek Turecek[1]; *[1]University of Washington, Seattle, WA*

8:30 - 10:30 am Thursday
POST-TRANSLATIONAL MODIFICATIONS: QUALITATIVE & QUANTITATIVE ANALYSIS
Session Chair: Kristina Hakansson (University of Michigan)
B405-407

ThOC am 08:30 **Strategies for High Throughput MS Analysis of Acid-Labile Phosphorylation**; Gemma Hardman[1]; Simon Perkins[1]; Philip Brownridge[1]; Andrew Jones[1]; Claire Eyers[1]; *[1]University of Liverpool, Liverpool, United Kingdom*

ThOC am 08:50 **Mass Spectrometry-Based Large-Scale and Precise Identification of Citrullinated Proteins from Complex Biological Samples**; Yatao Shi[1]; Zihui Li[2]; Xudong Shi[3]; Bin Wang[4]; Lingjun Li[2,4]; *[1]University of Wisconsin, Madison, WI; [2]Department of Chemistry, University of Wisconsin, Madison, WI; [3]Department of Surgery, School of Medicine and Public Health, University of Wisconsin, Madison, WI; [4]School of Pharmacy, University of Wisconsin, Madison, WI*

ThOC am 09:10 **ProteomeTools: Exploiting the Largest Collection of Synthetic Peptides Carrying Biologically Relevant Post-Translational Modifications for Proteome Research**; Daniel P Zolg[1]; Mathias Wilhelm[1]; Siegfried Gessulat[1,2]; Tobias Schmidt[1]; Michael Graber[1,3]; Jana Zecha[1]; Johannes Zerweck[4]; Tobias Knaute[4]; Hans-Christian Ehrlich[2]; Stephan Aiche[2]; Bernard Delanghe[5]; Andreas Huhmer[6]; Karsten Schnatbaum[4]; Ulf Reimer[4]; Bernhard Kuster[1,7,8]; *[1]Technical University of Munich, Freising, Germany; [2]SAP SE, Potsdam, Germany; [3]Ludwig-Maximilians-University Munich, Munich, Germany; [4]JPT Peptide Technologies GmbH, Berlin, Germany; [5]Thermo Fisher Scientific, Bremen, Germany; [6]Thermo Fisher Scientific, San Jose, CA; [7]Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany; [8]Center for Integrated Protein Science Munich, Freising, Germany*

ThOC am 09:30 **Critical Insight on Protein Oxidation Mapping by LC-MS/MS: Identification, Quantification, Artifacts, and Implications**; Qian Dong[1]; Yuxue Liang[1]; Xinjian Yan[1]; Stephen E. Stein[1]; *[1]NIST, Gaithersburg, MD*

ThOC am 09:50 **Integration of Lysine Modification Changes and Bioenergetic Phenotypes in Mouse Models of Cardiac Mitochondrial Protein Hyperacylation**; Paul A. Grimsrud[1]; Michael T. Davidson[1]; Kelsey H. Fisher-Wellman[2]; James A. Draper[1]; Ling Lai[3]; Matthew D. Hirschey[1]; Timothy R. Koves[1]; Daniel P. Kelly[3]; Deborah M. Muoio[1]; *[1]Duke University School of Medicine, Durham, NC; [2]East Carolina University Brody School of Medicine, Greenville, NC; [3]Perelman School of Medicine - University of Pennsylvania, Philadelphia, PA*

ThOC am 10:10 **Coupling Fluorescent-Activated Cell Sorting with LC-MRM-MS to Characterize Epi-Proteomic Signatures from Human Blood Cells**; Jeannie M Camarillo[1]; Suchitra Swaminathan[1]; Nebiyu A Abshiru[1]; Juliette A Morris[1]; Madeline A Zoltek[1]; Jacek W Sikora[2]; Paul M Thomas[2]; Neil L Kelleher[2]; *[1]Northwestern University, Chicago, IL; [2]Northwestern University, Evanston, IL*

8:30 - 10:30 am Thursday
DRUG DISCOVERY AND DEVELOPMENT : QUANTITATIVE ANALYSIS
Session Chair: Christopher Yu (Genentech)
B302-305

ThOD am 08:30 **Utility of a Novel Acoustic Mist Ionization Front End in Early Drug Discovery: Delivery of a HTP Biochemical Screen**; Arseniy M Belov[1]; Carl A Machutta[1]; Guofeng Zhang[1]; Joseph Kozole[1]; Jeffrey W Gross[1]; Melanie V Leveridge[1]; Luke Ghislain[2]; Sammy S Datwani[2]; Roland S Annan[1]; *[1]GlaxoSmithKline, Collegeville, PA; [2]Labcyte Inc., San Jose, CA*

ThOD am 08:50 **Quantitative Interactomics as a Tool for Drug Development**; James Bruce[1]; Juan D. Chavez[1]; Andrew Keller[1]; Jared P. Mohr[1]; Martin Mathay[1]; *[1]University of Washington, Genome Sciences, Seattle, WA*

ThOD am 09:10 **Overcoming ADA Interference by Using a Hybrid LC/MS/MS Method to Quantify a Therapeutic Protein in Human Plasma**; Jia Guo[1]; Dylan Sorensen[2]; Chad Christianson[3]; Tara O'Brien[3]; Leonor Newquist[1]; Kevin Kuang[1]; Ben Badillo[1]; Ryan Boyer[1]; Stephen Zoog[1]; Huiyu Zhou[1]; *[1]BioMarin Pharmaceutical Inc., Novato, CA; [2]Amgen, South San Francisco; [3]Alturas Analytics, Moscow, ID*

ThOD am 09:30 **Quantification of Convoluted Antibody and Antibody-Drug-Conjugate Modifications at the Intact and Middle-Down Level *via* ETD Fragments and Isotopically-Labeled Standards;** Joseph D Eschweiler[1]; Guillaume Tremintin[2]; Reika Campbell[1]; Julie L Heflin[1]; *[1]AbbVie Inc., North Chicago, IL; [2]Bruker Scientific, San Jose, CA*

ThOD am 09:50 **Benchmarking of HR/AM Instruments for Monitoring and Accurately Quantifying Trace-Level Host Cell Proteins Impurities in Therapeutic Proteins;** Joanna Bons[1]; Nicolas Pythoud[1]; Sarah Cianférani[1]; Christine Carapito[1]; *[1]Laboratoire de Spectrométrie de Masse BioOrganique, Université de Strasbourg, CNRS, IPHC UMR 7178, Strasbourg, France*

ThOD am 10:10 **Analysis and Characterization of Adeno Associated Virus by Charge Detection Mass Spectrometry;** Nicholas A. Lyktey[1]; Zachary C. Elmore[2]; Eric Walton[2]; Aravind Asokan[3]; Martin F. Jarrold[1]; *[1]Indiana University, Bloomington, IN; [2]Duke University, Durham, NC; [3]Duke University School of Medicine, Durham, NC*

8:30 - 10:30 am Thursday
SUPRAMOLECULAR AND MACROMOLECULAR COMPLEXES
Session Chair: Stacy D. Sherrod (Vanderbilt University)
B308-309

ThOE am 08:30 **Using Supramolecular Protein-Polymer Complexes to Probe Surface-Accessible Protein Residues;** Benqian Wei[1]; Selim Gerislioglu[2]; Jonathan P Williams[3]; Chrys Wesdemiotis[1]; *[1]The University of Akron, Akron, OH; [2]PPG, Allison Park, PA 15101; [3]Waters corporation, Wilmslow, United Kingdom*

ThOE am 08:50 **Data Integration and Mass Spectrometry for Solving Structures of Intrinsically Disordered Regions of Nuclear Receptors;** Mark Chance[1]; Janna Kiselar[1]; Sichun Yang[1]; *[1]Case Western Reserve University, Cleveland, OH*

ThOE am 09:10 **Relative Stabilities of Lipoprotein Subpopulations Determined by Charge Detection Mass Spectrometry;** Corinne A. Lutomski[1]; Tarick J. El-Baba[1]; David E. Clemmer[1]; Martin F. Jarrold[1]; *[1]Indiana University, Bloomington, IN*

ThOE am 09:30 **Probing Gas-Phase Unfolding Mechanism of Multimeric Protein Complexes by Native Top-Down Mass Spectrometry Using Electron Capture Dissociation and Ultraviolet Photodissociation;** Mowei Zhou[1]; Weijing Liu[1]; Ljiljana Pasa-Tolic[1]; Jared B. Shaw[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

ThOE am 09:50 **Identification and Quantitation of Heterodimer Species in Co-Formulated Protein Drugs by LC-MS-Based Approaches;** Tao Xing[1]; Yuetian Yan[1]; Shunhai wang[1]; Thomas J. Daly[1]; Ning li[1]; *[1]Regeneron Pharmaceuticals Inc., Tarrytown, NY*

ThOE am 10:10 **Towards a Comprehensive Landscape of 60S Ribosomal Biogenesis;** Carolin Sailer[1]; Jasmin Jansen[1]; Axel Reiser[2]; Jan Erzberger[3]; Florian Stengel[1]; *[1]University of Konstanz, Konstanz, Germany; [2]University of Stuttgart, Stuttgart, Germany; [3]UT Southwestern Medical Center, Dallas, TX*

8:30 - 10:30 am Thursday
CLINICAL ANALYSIS USING MS
Session Chair: Yu Bai (Peking University)
B312-314

ThOF am 08:30 **Development of Robust Spatial Metabolomics Tools for Cross-Site Analyses of Human Biopsies for Kidney Precision Medicine;** Dusan Velickovic[1]; Guanshi Zhang[2]; Arunima Bhattacharjee[1]; Jennifer Kyle[1]; Ryan Sontag[1]; Ljiljana Pasa-Tolic[1]; Theodore Alexandrov[3]; Kumar Sharma[2]; Christopher Anderton[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]University of Texas Health-San Antonio, San Antonio, TX; [3]European Molecular Biology Laboratory, Heidelberg, Germany*

ThOF am 08:50 **Quantitation of Cannabinoids in Breath Samples Using a Novel Derivatization LC-MS Assay with Ultrahigh Sensitivity;** Yiqi Ruben Luo[1]; Cassandra Yun[1]; Kara L Lynch[1]; *[1]University of California, San Francisco, CA*

ThOF am 09:10 **Development of Automated, Multiplexed PI3K p110α, PTEN, and AKT 1+2 Assays for Tumor-Tissue Samples Using Immuno-MALDI Mass Spectrometry (iMALDI);** Bjorn Frohlich[1]; Robert Popp[1]; Rene Zahedi[2]; Andre LeBlanc[2]; Yassene Mohammed[1, 3]; Adriana Aguilar-Mahecha[4]; Oliver Poetz[5]; Mark Basik[6]; Gerald Batist[6]; Christoph H. Borchers[1, 2, 6, 7]; *[1]University of Victoria-Genome BC Proteomics Centre, Victoria, BC; [2]Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; [3]Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; [4]Segal Cancer Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; [5]NMI Natural and Medical Sciences Institute at the University of Tuebingen, Tuebingen, Germany; [6]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC; [7]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC*

ThOF am 09:30 **Paper Spray Ionization-Mass Spectrometry (PSI-MS) for the Simultaneous Quantification of Five Tri-azole Anti-fungal Agents from Plasma Samples;** Lindsey M Kirkpatrick[1, 2]; Christine L Skaggs[3]; Greta J Ren[3]; Nicholas E Manicke[4]; *[1]Indiana University School of Medicine, Pediatric Infectious Disease, Indianapolis, IN; [2]James Whitcomb Riley Hospital for Children, Indianapolis, Indiana; [3]Department of Chemistry and Chemical Biology, Indiana University-Purdue University Indianapolis, Indianapolis, IN; [4]Department of Chemistry and Chemical Biology, Forensic and Investigative Sciences Program, Indiana University-Purdue University Indianapolis, Indianapolis, IN*

ThOF am 09:50 **Molecular Analysis of Endometriosis to Aid in Surgical Resection Using the Laparoscopic MasSpec Pen;** Clara Feider[1]; Jialing Zhang[1]; John Q. Lin[1]; Marta Sans[1]; Suzanne Ledet[2]; Katherine Sebastian[2]; Michael T. Breen[3]; Livia S. Eberlin[1]; *[1]The University of Texas, Austin, TX; [2]Seton Medical Center, Austin, TX; [3]Dell Medical School at The University of Texas, Austin, TX*

ThOF am 10:10 **Quality Control Considerations for Targeted MRM on Dried Blood Microsamples for Early Prediction of Cardiac Events;** Kelly Njine Mouapi[1]; Irene Van Den Broek[1]; Mitra Mastali[1]; Qin Fu[1]; Vidya Venkatraman[1]; Noel Bairey Merz[2]; Brennan Spiegel[3]; Jennifer Van Eyk[1, 2]; *[1]Advanced Clinical Biosystems Research Institute, The Smidt Heart Institute, Cedars-Sinai Medical Center, Los Angeles, CA; [2]Barbra Streisand Women's Heart Center, The Smidt Heart Institute, Cedars-Sinai Medical Center, Los Angeles, CA; [3]Cedars Sinai Center for Outcomes Research and Education (CS-CORE), Cedars-Sinai Medical Center, Los Angeles, CA*

8:30 - 10:30 am Thursday
STABLE ISOTOPE LABELING IN MS: APPLICATIONS
Session Chair: Chengli Zu (Corteva Agriscience)
Auditorium, Bldg A

ThOG am 08:30 **Probing Metabolic Pathways during Early Embryonic Development Using Stable Isotope Labeling and Single-Cell Mass Spectrometry**; Erika Portero[1]; Aleena J Andrews[1]; Peter Nemes[1]; *[1]University of Maryland, College Park, MD*

ThOG am 08:50 **A Boosting to Amplify Signal with Isobaric Labeling (BASIL) Strategy for Comprehensive Quantitative Phosphoproteomic Characterization of Small Populations of Cells**; Chia-Feng Tsai[1]; Lian Yi[1]; Ercument Dirice[2]; Adam C. Swensen[1]; Jing Chen[3]; Marina A. Gritsenko[1]; Rosalie K. Chu[4]; Paul D. Piehowski[1]; Richard D. Smith[1,4]; Karin D. Rodland[1]; Clayton E. Mathews[3]; Rohit N. Kulkarni[2]; Wei-Jun Qian[1]; Tao Liu[1]; *[1]Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; [2]Section of Islet Cell Biology and Regenerative Medicine, Joslin Diabetes Center and Harvard Medical School, Boston, MA; [3]Department of Pathology, Immunology, and Laboratory Medicine, University of Florida, Gainesville, FL; [4]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA*

ThOG am 09:10 **Quantitative Analysis of the Fetal Tissue Translatome by Mass Spectrometry Reveals Temporal and Tissue-Specific Regulatory Networks *in utero***; Josue Baeza[1]; Coons E Barbara[2]; William Peranteau[2]; Benjamin A. Garcia[1]; *[1]University of Pennsylvania, Philadelphia, PA; [2]Children's Hospital of Philadelphia, Philadelphia, PA*

ThOG am 09:30 **Spatial Isotope Tracer Metabolomics to Study 13C Labeled Metabolite Distribution in 3D Tumor Spheroid Cell Culture**; Prasad Phapale[1]; Mariia Naumenko[1,2]; Karin Mitosch[1,3]; Theodore Alexandrov[1,2,4]; *[1]EMBL, Heidelberg, Heidelberg, Germany; [2]Metabolomics Core Facility, European Molecular Biology Laboratory, Heidelberg, Germany, Heidelberg, Germany; [3]Genome Biology Unit, European Molecular Biology Laboratory, Heidelberg, Germany, Heidelberg, Germany; [4]UCSD, San Diego, CA*

ThOG am 09:50 **DIA and DDA MS for Profiling the Cancer Borealis Neuropeptidome and Peptidomic Changes Resulting from Food Intake**; Kellen DeLaney[1]; Lingjun Li[1]; *[1]University of Wisconsin, Madison, WI*

ThOG am 10:10 **Determining the Metabolic Fate of Monosaccharides in the Glycocalyx through Stable Isotope Labeling**; Maurice Wong[1]; Gege Xu[1]; Mariana Barboza[1]; Carlito Lebrilla[1]; *[1]University of California, Davis, CA*

8:30 - 10:30 am Thursday
EXPOSOMICS, TOXICOLOGY, AND HUMAN HEALTH
Session Chair: Jon R. Sobus (US EPA)
A411-412

ThOH am 08:30 **Wastewater Impacts on Drinking Water: Hospital and Energy-Related Wastes and the Formation of Higher-Toxicity Disinfection By-Products**; Hannah Liberatore[1]; Danielle C. Westerman[1]; Caroline O. Granger[1]; Amy A. Cuthbertson[1]; Joshua M. Allen[1]; Michael J Plewa[2]; Elizabeth D Wagner[2]; Kelly D Good[3]; Amy McKenna[4]; Chad R. Weisbrod[4]; Jerry A. Zweigenbaum[5]; Jeanne M. VanBriesen[3]; Susan D. Richardson[1]; *[1]University of South Carolina, Columbia, SC; [2]University of Illinois Urbana-Champaign, Urbana, IL; [3]Carnegie Mellon University, Pittsburgh, PA; [4]National High Magnetic Field Laboratory, Tallahassee, FL; [5]Agilent Technologies, Inc., Wilmington, DE*

ThOH am 08:50 ***In vitro* Hepatic Clearance of Per- and Polyfluoroalkyl Substances (PFAS)**; David M. Crizer[1]; Tahja M. Harris[1]; Paul E. Dunlap[1]; Julie R. Rice[1]; Stephen S. Ferguson[1]; Michael J. DeVito[1]; *[1]National Toxicology Program/NIEHS/NIH, Research Triangle Park, NC*

ThOH am 09:10 **HRMS-Based Metabolomics Strategy for Comprehensively Screening Biomarkers of Phthalate Exposure and their Applications**; Jing-fang Hsu[1]; Chia-Lung Shih[2]; Pao-Chi Liao[2]; *[1]National Health Research Institutes, Miaoli County, Taiwan; [2]National Cheng Kung University, Tainan, Taiwan*

ThOH am 09:30 **An Algorithm (wSIM-CITY) for Gas Phase Fractionated (GPF) MS/MS2 Data Independent Acquisition (DIA) and Application to Neutral Loss DNA Adductomics.**; Scott J Walmsley[1,2]; Jinshu Guo[1,3]; Peter W. Villalta[1]; Robert Turesky[1,3]; Jinhua Wang[1,2]; *[1]Masonic Cancer Center, University of Minnesota, Minneapolis, MN; [2]Institute for Health Informatics, University of Minnesota, Minneapolis, MN; [3]Dept. of Medicinal Chemistry, College of Pharmacy, Minneapolis, MN*

ThOH am 09:50 **Signatures of Ambient Exposure to Benzene and Other Air Pollutants in the Human Serum Albumin Cys34 Adductome**; Joshua W Smith[1]; Robert N O'Meally[1]; Thomas W Kensler[1,2]; Robert N Cole[1]; John D Groopman[1]; *[1]Johns Hopkins University, Baltimore, MD; [2]Fred Hutchinson Cancer Research Center, Seattle, WA*

ThOH am 10:10 **Multi-omics Investigation Reveals Benzalkonium Chloride Disinfectants Alter Sterol and Lipid Homeostasis in the Mouse Neonatal Brain**; Josi M. Herron[1]; Kelly M. Hines[1]; Hideaki Tomita[1]; Ryan P. Seguin[1]; Julia Y. Cui[1]; Libin Xu[1]; *[1]University of Washington, Seattle, WA*

10:30 am - 2:30 pm Thursday

THURSDAY POSTER SESSION
Poster/Exhibit Hall ground level
Lunch concessions are open 11:00 am - 2:00 pm

Odd-number posters present:
10:30 am - 11:30 am PLUS 12:30 - 2:30 pm

Even-number posters present:
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Poster Pick-Me-Up Snacks served at 1:30 pm



2:30 - 4:30 pm Thursday
INFORMATICS: PEPTIDE AND PROTEIN IDENTIFICATION, PROTEOMICS
Session Chair: Anna Ivanova (Emory University)
Murphy Ballroom, Bldg B, Level 5

ThOA pm 02:30 **From Single Software Tools to Fully Reproducible Workflows for the Analysis of Protein Mass Spectrometry Data**; Johannes Griss[1,2]; Goran Vinterhalter[3]; Iustinian Olaru[4]; Veit Schwämmle[4]; *[1]Medical University of Vienna, Vienna, Austria; [2]EMBL-EBI, Hinxton, United Kingdom; [3]University of Belgrade, Belgrade, Serbia; [4]University of Southern Denmark, Odense, Denmark*

ThOA pm 02:50 **A Novel Computational Approach for Simultaneous Identification of Protein-RNA and Protein-DNA Interactions from XL-MS Data**; Timo Sachsenberg[1]; Alexandra Stützer[2]; Aleksandar Chernev[2]; Eugen Netz[3]; Tjeerd Dijkstra[4]; Henning Urlaub[2,5]; Oliver Kohlbacher[1,6,7,8]; *[1]University of Tübingen, Tübingen, Germany; [2]Max Planck Institute for biophysical chemistry, Göttingen, Germany; [3]Max Planck Institute for Developmental Biology, Tuebingen, Germany; [4]Max Planck Institute for Developmental Biology, Tuebingen, Germany; [5]University Medical Center Goettingen (UMG), Goettingen, Germany; [6]Biomolecular Interactions, Max Planck Institute for Developmental Biology, Tübingen, Germany; [7]Institute for Translational Bioinformatics, University Hospital Tübingen, Tübingen, Germany; [8]Quantitative Biology Center, University of Tübingen, Tübingen, Germany*

ThOA pm 03:10 **PRISM: Pattern-Based, Assumption-Free Protein Identification**; Joris Van Houtven[1,2,3]; Kurt Boonen[1,3]; Geert Baggerman[1,3]; Kris Laukens[4,5]; Jef Hooyberghs[1,6]; Dirk Valkenborg[2,3]; *[1]Flemish Institute for Technological Research (VITO), Mol, Belgium; [2]University of Hasselt, Diepenbeek, Belgium; [3]Centre for Proteomics, University of Antwerp, Antwerp, Belgium; [4]biomedical informatics network Antwerpen (biomina), University of Antwerp, Antwerp, Belgium; [5]Dept. Mathematics & Computer Science, University of Antwerp, Antwerp, Belgium; [6]Theoretical Physics, Hasselt University, Diepenbeek, Belgium*

ThOA pm 03:30 **A "Divide and Conquer" Approach to Address Peptide-Spectrum Matching Challenges of Large Sequence Databases in Next-Generation Proteomic Applications**; Praveen Kumar[1,2]; James E. Johnson[3]; Thomas McGowan[3]; Subina Mehta[2]; Ray Sajulga[2]; Shane Hubler[1]; Caleb Easterly[2]; Matthew C. Chambers[5]; Pratik Jagtap[2]; Timothy J. Griffin[2]; *[1]Bioinformatics and Computational Biology, University of Minnesota-Rochester, Rochester, MN; [2]Biochemistry, Molecular Biology, and Biophysics, University of Minnesota, Minneapolis, MN; [3]Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, MN; [4]Rhapsody Data, LLC., Madison, WI; [5]Vanderbilt University, Nashville, TN*

ThOA pm 03:50 **Proteomic Data Commons (PDC): A Node in the NCI Cancer Research Data Commons**; Paul A Rudnick[1]; Ratna R. Thangudu[2]; Michael Holck[2]; Deepak Singhal[2]; Karen A. Ketchum[2]; Nathan J. Edwards[3]; Christopher R. Kinsinger[1]; Izumi Hinkson[5]; Lei Ma[2]; Maya Zuhl[2]; Yi Xin[2]; Padmini Chilappagari[2]; Anand Basu[2]; Michael J MacCoss[6]; *[1]Spectragen Informatics, Bainbridge Island, WA; [2]ESAC, Inc., Rockville, MD; [3]Georgetown University Medical Center, Washington, DC; [4]National Cancer Institute, Bethesda, MD; [5]National Cancer Institute @ Frederick, Frederick, MD; [6]University of Washington, Genome Sciences, Seattle, WA*

ThOA pm 04:10 **Detection of Cancer Mutations in Proteomics Data with a Cloud Search Engine**; Conor Jenkins[1]; Megan Rigby[2]; Amol Prakash[3]; Benjamin Orsburn[2]; *[1]Hood College Bioinformatics Program, Frederick, MD; [2]National Cancer Institute @ Frederick, Frederick, MD; [3]Optys Tech Corporation, Shrewsbury, MA*

2:30 - 4:30 pm Thursday
MICROORGANISMS AND THE MICROBIOME
Session Chair: Neha Garg (Georgia Institute of Technology)
B401-402

ThOB pm 02:30 **Identification of Individual Bacteria in Polymicrobial Samples *via* Membrane Glycolipids**; David R. Goodlett[1]; Alison J. Scott[1]; Sung Hwan Yoon[1]; So Young Ryu[2]; Dusan Velickovic[3]; Rene Boiteau[4]; Robert K. Ernst[1]; Ljiljana Pasa-Tolic[3]; *[1]University of Maryland, Baltimore, MD; [2]University of Nevada, Reno, NV; [3]Pacific Northwest National Laboratory, Richland, WA; [4]Oregon State University, Crovalis, OR*

ThOB pm 02:50 **Approaches to Accurate Chemical Constitutional Analysis in Untargeted Microbial Natural Products Research**; Roger Linington; *Simon Fraser University, Burnaby, BC*

ThOB pm 03:10 **Evaluation of a Biofilm Inhibitor Using Imaging Mass Spectrometry Raises Questions about Potential Therapeutic Strategies**; Alanna R Condren[1]; Lisa Kahl[2]; Manuel Banzhaf[3]; Lars Dietrich[2]; Laura Sanchez[1]; *[1]University of Illinois, Chicago, IL; [2]Columbia University, New York, NY; [3]University of Birmingham, Birmingham, United Kingdom*

ThOB pm 03:30 **Metabolomics Activity Screening Identifies Immunomodulating Host-Microbiome Metabolites in Inflammatory Bowel Disease** ; J. Rafael Montenegro-Burke[1]; Bernard P. C. Kok[1]; Carlos Guijas[1]; Enrique Saez[1]; Dennis Wolan[1]; Gary Siuzdak[1]; *[1]The Scripps Research Institute, La Jolla*

ThOB pm 03:50 **LC-MS/MS-based Metabolomics Reveals Inhibition Effect of Gut Microbiota-Derived Metabolites on Lipid Accumulation in Hepatocytes**; Qiang Lyu[1]; Hsin-Bei Tsou[1]; Hsin-Yuan Chang[1]; Yin-Hsuan Huang[1]; Hsiao-Li Chuang[2]; Cheng-Chih Hsu[1]; *[1]National Taiwan University, Taipei, Taiwan; [2]National Laboratory Animal Center, Taipei, Taiwan*

ThOB pm 04:10 **Discovering Small Molecule Products of Biosynthetic Gene Clusters by Integrating Metagenomics and Mass Spectrometry**; Liu Cao[1]; Egor Shcherbin[2]; Hosein Mohimani[1]; *[1]Computational Biology Department, School of Computer Science, Carnegie Mellon University, Pittsburgh, PA; [2]National Research University Higher School of Economics, St. Petersburg, Russia*

2:30 - 4:30 pm Thursday
QUANTITATIVE PROTEOMICS IN SYSTEMS BIOLOGY
Session Chair: Susan E. Abbatiello (Northeastern University)
B405-407

ThOC pm 02:30 **Profiling the HSP90 Clientele in EGFR Mutant Cancer Cells**; Jason Liang[1]; Trent Hinkle[1]; Erik Verschueren[1]; Shiva Malek[2]; Donald S. Kirkpatrick[1]; *[1]Department of Microchemistry, Proteomics and Lipidomics, Genentech Inc., South San Francisco, CA; [2]Department of Discovery Oncology, Genentech Inc., South San Francisco, CA*

ThOC pm 02:50 **Investigating the Role of Histone H2A Proteolysis during Stem Cell Differentiation and Its Consequence in Nucleosome Stability**; Mariel Coradin[1]; Kelly R. Karch[1]; Simone Sidoli[1]; Benjamin A. Garcia[1]; *[1]University of Pennsylvania, Philadelphia, PA*

ThOC pm 03:10 **Quantitative Time-Course Profiling of Sorafenib-Treated Hepatocellular Carcinoma (HCC) Cells Through Phosphoproteome Analysis**; Emily Werth[1]; Presha Rajbhandari[1]; Brent R Stockwell[1]; Lewis M. Brown[1]; *[1]Columbia University, New York, NY*

ThOC pm 03:30 **A Versatile Lentiviral Delivery Toolkit for Proximity-dependent Biotinylation in Diverse Cell Types**; Payman Samavarchi-Tehrani[1]; Hala Abdouni[1]; Reuben Samson[1]; Cassandra Wong[1]; Anne-Claude Gingras[1,2]; *[1]Lunenfeld-Tanenbaum Research Institute, Sinai Health System, Toronto, ON; [2]University of Toronto, Toronto, ON*

ThOC pm 03:50 **Proteomic Analysis of Sorted Mouse Embryonic Stem Cells to Decipher Sub-populations**; Molly P. Lowndes[1,2]; Joshua M. Brickman[2]; Michael L. Nielsen[1]; *[1]Novo Nordisk Foundation Center for Protein Research, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark; [2]Novo Nordisk Foundation Center for Stem Cell Biology, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark*

ThOC pm 04:10 **Illuminating the Dark Kinome: Defining Kinase-Substrate Relationships Using Targeted Protein Degradation and Phosphoproteomics**; Rufus Hards[1]; Ian LaCroix[1]; Arminja N Kettenbach[1]; Andrew Holland[2]; Scott A. Gerber[1]; *[1]Geisel School of Medicine at Dartmouth, Lebanon, NH; [2]Johns Hopkins, Baltimore, MD*

2:30 - 4:30 pm Thursday
COVALENT LABELING AND CHEMICAL CROSSLINKING
Session Chair: Florian Stengel (University of Konstanz)
B302-305

ThOD pm 02:30 **PhoX - an IMAC-enrichable Crosslinking Reagent**; Barbara A. Steigenberger[1,2]; Roland J. Pieters[3]; Albert J.R. Heck[1,2]; Richard A. Scheltema[1,2]; *[1]Biomolecular Mass Spectrometry and Proteomics, Bijvoet Center for Biomolecular Research and Utrecht Institute of Pharmaceutical Sciences, Utrecht University, Utrecht, Netherlands; [2]Netherlands Proteomics Center, Utrecht, Netherlands; [3]Department of Chemical Biology & Drug Discovery, Utrecht University, Utrecht, Netherlands*

ThOD pm 02:50 **Developing Cross-linking Mass Spectrometry (XL-MS) to Delineate Protein Interaction Landscapes in Living Cells**; Andrew Wheat[1]; Clinton Yu[1]; Xiaorong Wang[1]; Lan Huang[1]; *[1]University of California, Irvine, CA*

ThOD pm 03:10 **Chemical Cross-Linking and Covalent Labelling Provide Insights into the Protein Organisation of Synaptic Vesicle Membranes**; Sabine Wittig[1]; Marie Barth[1]; Marcelo Ganzella[2]; Julia Preobraschenski[2]; Susann Kostmann[1]; Angel Perez-Lara[2]; Reinhard Jahn[2]; Carla Schmidt[1]; *[1]HALOmem, Martin Luther University Halle-Wittenberg, Halle / Saale, Germany; [2]MPI for Biophysical Chemistry, Department of Neurobiology, Göttingen, Germany*

ThOD pm 03:30 **Chemical Protein-RNA Cross-Linking Coupled with Mass Spectrometry – from Proteins to Cells**; Alexander Wulf[1]; Luisa M Welp[1]; Seychelle Vos[1]; Sven Johansson[2]; Timo Sachsenberg[3]; Ralf Ficner[2]; Oliver Kohlbacher[3]; Patrick Cramer[1]; Henning Urlaub[1,4]; *[1]Max Planck Institute for biophysical chemistry, Göttingen, Germany; [2]University of Goettingen, Institute for Microbiology and Genetics, Goettingen, Germany; [3]University of Tubingen, Tubingen, Germany; [4]University Medical Center Goettingen (UMG), Goettingen, Germany*

ThOD pm 03:50 **Structure Determination of Neurodegenerative Disease-Related Misfolded Protein Aggregegrates by Short-Distance Crosslinking Constraint-Guided Discrete Molecular Dynamics (CL-DMD)**; Evgeniy V. Petrotchenko[1]; Jason J. Serpa[2]; Konstantin I. Popov[3]; Nikolay V. Dokholyan[4]; Christoph H. Borchers[1,2,5,6]; *[1]Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; [2]University of Victoria-Genome BC Proteomics Centre, Victoria, BC; [3]Department of Biochemistry and Biophysics, University of North Carolina, Chapel Hill, NC; [4]Departments of Pharmacology, and Biochemistry and Molecular Biology, Pennsylvania State College of Medicine, Hershey, PA; [5]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; [6]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC*

ThOD pm 04:10 **Multidimensional Cross-Linking with a Tetra-Reactive Cross-Linker**; Jared P. Mohr[1]; Juan D. Chavez[1]; James E. Bruce[1]; *[1]University of Washington, Genome Sciences, Seattle, WA*

2:30 - 4:30 pm Thursday
PLANT "OMICS"
Session Chair: Michael R. Sussman (University of Wisconsin)
B308-309

ThOE pm 02:30 **Elucidation of Molecular Switches Regulating Plant C3to CAM Transition Using Integrative Transcriptomics, Proteomics and Metabolomics**; Sixue Chen; *University of Florida, Gainesville, FL*

ThOE pm 02:50 **Digging Deep into the Transcriptome, Proteome and Phosphoproteome of *Arabidopsis thaliana***; Julia Mergner[1]; Martin Heinrich Frejno[1]; Markus List[1]; Maxim Messerer[2]; Daniel Lang[2]; Stefan Altmann[2]; Philipp Cyprys[3]; Toby Mathieson[4]; Klaus Mayer[2]; Pascal Falter-Braun[2]; Stefanie Sprunck[3]; Jan Baumbach[1]; Claus Schwechheimer[1]; Bernhard Kuster[1]; *[1]Technical University of Munich, Freising, Germany; [2]Helmholtz Center Munich, Neuherberg, Germany; [3]University of Regensburg, Regensburg, Germany; [4]Cellzome, a GSK company, Heidelberg, Germany*

ThOE pm 03:10 **Automated High-throughput Metabolic Analysis of Single Cells by Fiber Based Laser Ablation Electrospray Ionization Mass Spectrometry**; Sylwia Stopka[1]; Ellen A Wood[1]; Rikkita Khattar[1]; Beverly J Agtuca[2]; Christopher R Anderton[3]; David W Koppenaal[3]; Ljiljana Pasa-Tolic[3]; Gary Stacey[2]; Akos Vertes[1]; *[1]The George Washington University, Washington, DC; [2]University of Missouri, Columbia, MO; [3]Pacific Northwest National Laboratory, Richland, WA*

ThOE pm 03:30 **Establishing and Applying Mass Spectrometric Tools to Measure Levels and 13C-Labeling Kinetics of Metabolites in *Camelina sativa* Leaves and Seeds**; Yuan Xu[1]; Bibin Paulose[1]; Hesham Abdullah[1]; Danny Schnell[1]; Yair Shachar-Hill[1]; *[1]Michigan State University, East Lansing, MI*

ThOE pm 03:50 **Comparing Proteomic Changes during PAMP Responses and MKP1-Requiring Genetic Pathways**; Laura A Greeley[1]; Gabrielle Rupp[1]; Scott C Peck[1]; *[1]University of Missouri, Columbia, MO*

ThOE pm 04:10 **Novel Bioactive Cyclotide Scaffolds in *Viola inconspicua***; Nicole C Parsley[1]; Patric W Sadecki[1]; Conrad J Hartmann[1]; Leslie M Hicks[1]; *[1]UNC Chapel Hill, Durham, NC*

2:30 - 4:30 pm Thursday
ION MOBILITY: STRUCTURE
Session Chair: Francisco Fernandez Lima (Florida International University)
B312-314

ThOF pm 02:30 **Mechanism of Amyloid Assembly: Prion-like Cross Talk betweeen Disease Agents of Alzheimer's, Amyotrophic Lateral Sclerosis(ALS) and Type 2 Diabetes**; Shruti Arya[1]; Veronica Laos[1]; Michael T. Bowers[1]; *[1]University of California, Santa Barbara, CA*

ThOF pm 02:50 **Ion Mobility Spectrometry-Mass Spectrometry Reveals Subtle Differences in Structure and Stability in Wild-Type Versus Point-Mutated Variants of Chymotrypsin Inhibitor 2**; Shannon A. Raab[1]; Tarick J. El-Baba[1]; Daniel W. Woodall[1]; Wen Liu[2]; Yang Liu[2]; Arthur Laganowsky[2]; David H. Russell[2]; David E. Clemmer[1]; *[1]Indiana University, Bloomington, IN; [2]Texas A&M University, College Station, TX*

ThOF pm 03:10 **Combining Solution Thermal Melting with IMS-MS Analysis to Investigate the Stability Effects of Ligand Interactions in Nucleic Acid Complexes**; Rebecca J. D'Esposito[1, 2]; Daniele Fabris[1, 2]; *[1]University at Albany, Albany, NY; [2]The RNA Institute, University at Albany, Albany, NY*

ThOF pm 03:30 **ESI/ESI Ion/Ion Reactions in the Traveling Wave Trap of an Ion Mobility/Mass Spectrometer for Gas-Phase Structure and Sequencing**; Veronica V. Carvalho[1]; Lyndon E. L. Keeling[1]; Rebecca L. Cain[1]; Griffin W. Dowell[1]; Prabhnoor S. Nagry[1]; Lindsay J. Morrison[2]; Jeffery M. Brown[3]; Ian K. Webb[1]; *[1]Indiana University Purdue University Indianapolis, Indianapolis, IN; [2]Waters Corporation, Beverly, MA; [3]Waters Corporation, Wilmslow, United Kingdom*

ThOF pm 03:50 **Delineation of Structural Isomers by Isotopic Shifts in High-Field Ion Mobility Spectra: Element-Specific Multidimensional Fingerprints**; Pratima Pathak[1]; Matthew A. Baird[1]; Gordon A. Anderson[2]; Alexandre A. Shvartsburg[1]; *[1]Wichita State University, Wichita, KS; [2]GAA Custom Engineering, LLC, Benton City, WA*

ThOF pm 04:10 **Towards Deciphering Tertiary Structures of Protein Glycoforms Using Tandem Trapped Ion Mobility Spectrometry-Mass Spectrometry**; Mengqi Chai[1]; Tyler C Cropley[1]; Fanny C Liu[1]; Christian Bleiholder[1]; *[1]Florida State University, Tallahassee, FL*

2:30 - 4:30 pm Thursday
INSTRUMENTATION: INNOVATIONS IN MASS ANALYZERS
Session Chair: Lissa Anderson (NHMFL-FSU)
Auditorium, Bldg A

ThOG pm 02:30 **Initial Experimental Characterization of the New Type of FT-Mass Spectrometer Based on Multielectrode Harmonized Kingdon Traps with Different Ion Sources**; Eugene (evgeny) Nikolaev[1]; Oleg Kharybin[1]; Gleb Vladimirov[1]; *[1]Skolkovo Institute of Science and Technology, Moscow Region, Russian Federation*

ThOG pm 02:50 **A Tandem Multi-Quadrupole Ion Trap (MultiQ-IT) Electrospray Interface for an Orbitrap Mass Spectrometer**; Andrew N. Krutchinsky[1]; Kelly R. Molloy[1]; Brian T. Chait[1]; *[1]The Rockefeller University, New York, NY*

ThOG pm 03:10 **Implementation of Ion-Ion Proton Transfer (IIPT) Reactions on a Modified Orbitrap Tribrid Mass Spectrometer with Increased Ion-Ion Reaction Capacity**; Christopher Mullen[1]; John E.P. Syka[1]; Lee Early[1]; Romain Huguet[1]; Jeffrey Shabanowitz[2]; Donald F. Hunt[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]University of Virginia, Charlottesville, VA*

ThOG pm 03:30 **Mirror Switching for Ion Isolation in a Fourier Transform Electrostatic Ion Trap Mass Spectrometer**; Joshua Johnson[1]; Gregory S. Eakins[1]; Scott A McLuckey[1]; *[1]Purdue University, West Lafayette, IN*

ThOG pm 03:50 **Digital Mass Filter Analysis Provides New Ways of Enhancing Sensitivity and Resolution**; Bojana Opacic[1]; Adam P. Huntley[1]; Peter T. A. Reilly[1]; *[1]Washington State University, Pullman, WA*

ThOG pm 04:10 **Nanomechanical Resonators based Charge Independent MS of Synthetic and Natural Nanoparticles in the 10-100 MDa Mass Range**; Christophe Masselon[1]; Shawn Fostner[2]; Sergio Dominguez-Medina[1]; Martial Defoort[2]; Emeline Verhnes[3]; Szu-Hsueh Lai[1]; Bogdan Vysotskyi[2]; Kavya Clement[1]; Thomas Alava[2]; Mohammad Abdul Halim[1]; Pascale Boulanger[3]; Sebastien Hentz[2]; *[1]Univ. Grenoble Alpes, CEA, Inserm, BIG-BGE, 38000 Grenoble, France; [2]Univ. Grenoble Alpes, CEA, LETI, 38000 Grenoble, France; [3]Univ Paris Sud, Univ. Paris Saclay, CEA, CNRS, I2BC, 91198 Gif sur Yvette, France*

2:30 - 4:30 pm Thursday
FUNDAMENTALS: ION ACTIVATION AND DISSOCIATION
Session Chair: Edwin De Pauw (University of Liege)
A411-412

ThOH pm 02:30 **Proton Transfer Reactions and Parallel Ion Parking for Intact Protein Analysis on a 21 T FT-ICR Mass Spectrometer**; Chad R. Weisbrod[1]; Lissa C. Anderson[1]; Jeffrey Shabanowitz[2]; Donald F. Hunt[2]; Christopher L. Hendrickson[3]; *[1]National High Magnetic Field Laboratory, Tallahassee, FL; [2]University of Virginia, Charlottesville, VA; [3]National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL*

ThOH pm 02:50 **Combining Ion Mobility Mass Spectrometry with Photoactivation – Lighting the Way to Conformer Analysis**; Rachelle L Black[1]; Alina Theisen[2]; Lennart Remakers[1]; Lukasz Migas[1]; Jeffery M Brown[3]; Bruno Bellina[1]; Perdita Barran[1]; *[1]Manchester Institute of Biotechnology, University of Manchester, United Kingdom; [2]University of Warwick, Coventry, United Kingdom; [3]Waters Corporation, Wilmslow, United Kingdom*

ThOH pm 03:10 **Characterization of Native Proteins with Activation Electron Transfer Dissociation (AI-ETD)**; Jean M Lodge[1]; Dain Ryan Brademan[2]; Michael S Westphall[3]; Joshua J Coon[2, 3, 4, 5]; *[1]University of Wisconsin, Madison, WI; [2]Department of Chemistry, University of Wisconsin, Madison, WI; [3]Genome Center of Wisconsin, Madison, WI; [4]Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; [5]Morgridge Institute for Research, Madison, WI*

ThOH pm 03:30 **Understanding Ionization and Fragmentation within the Solution Cathode Glow Discharge Ionization Source *via* Thermometer Molecule Analysis**; Courtney Walton[1]; Brian T. Molnar[1]; Judy Wu[1]; Jacob T. Shelley[1]; [1]*Rensselaer Polytechnic Institute, Troy, NY*

ThOH pm 03:50 **Structures, Binding Energetics, and Dissociation Dynamics of Imidazolium-Based Ionic Liquid Clusters**; Mary T Rodgers[1]; Harrison Roy[2]; [1]*Wayne State University, Detroit, MI;* [2]*Wayne State University, Detroit, MI*

ThOH pm 04:10 **A Novel Radical Ion Dissociation Technique for MS Characterization of RNA**; Giovanni Calderisi[1]; Kathrin Breuker[1]; [1]*University of Innsbruck, Innsbruck, Austria*

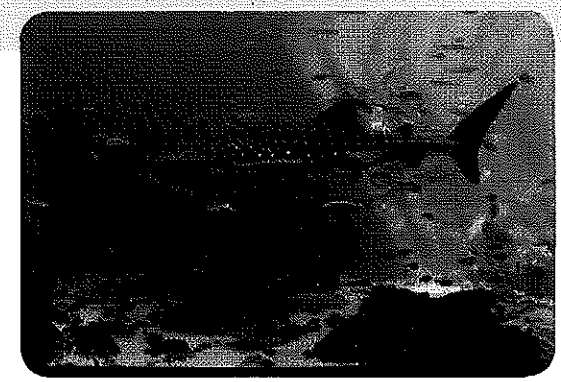
4:45-5:30 pm Thursday
PLENARY LECTURE
Presiding: Susan Richardson (University of South Carolina)
Murphy Ballroom, Bldg B, Level Five



Chemistry of Food and Soft Drinks

Lilly D'Angelo
Global Food & Beverage Technology Associates

6:30-9:30 pm Thursday
CLOSING EVENT
Georgia Aquarium
Advance purchase ticket is required ($40).
Tickets available for purchase through Monday at 12pm noon only.







POSTER OVERVIEW

Poster Presentation Schedule
Odd-number posters present: 10:30 am - 11:30 am PLUS 12:30 – 2:30 pm
Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm

MONDAY POSTERS

Set up all Monday posters
7:00 - 8:00 am

Odd-numbered posters present
10:30 - 11:30 am PLUS 12:30 - 2:30 pm

Even-numbered posters present
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Remove all Monday posters
7:00 - 8:00 pm

Biomarkers: Quantitative Analysis I 001-032
Biomolecular Structure Analysis: Chemical Crosslinking and Covalent Labeling I 033-060
Clinical Analysis I 061-083
Drug Metabolism: Qualitative & High Throughput Analysis 084-098
Drug and Metabolite Analysis: Novel Approaches for Dried Biological Samples 099-103
Energy: Biofuels and Algae 104-113
Environmental: Exposomics 114-130
Environmental: General I 131-161
Epigenetic Modifications 162-174
Food Safety I 175-200
Forensics I 201-229
Fundamentals: Ion Activation/Dissociation 230-255
Fundamentals: Ion Molecule, Ion/Ion, Ion/Electron Interactions 256-263
Fundamentals: Ion Spectroscopy 264-275
Fundamentals: Metal Ion Cationization, Metal-Ligand Interactions, Catalysis 276-282
Fundamentals: Molecular Modeling / Quantum Mechanical Calculations 283-291
H/D Exchange: Hardware, Software and Methodology 292-309
High Mass Accuracy/High Performance MS: Applications and Instrumentation 310-331
Imaging MS: Computational Methods and Analysis 332-342
Imaging MS: Instrumentation 343-359
Informatics: Algorithms and Statistical Advances I 360-382
Informatics: Peptide ID and Quantification 383-422
Informatics: Workflow and Data Management 423-445
Instrumentation: New Developments in Ionization and Sampling I 446-469
Instrumentation: New Developments in Mass Analyzers 470-494
Lipids: Profile Analysis 495-529
Lipids: Targeted and Quantitative Analysis 530-558
Metabolomics: Identification of Unknown Metabolites 559-576
Peptides: Sequence Analysis 577-584
Peptidomics 585-598
Phosphopeptides: Enrichment Methods 599-603
Plant "omics" 604-626
Polymers 627-639
Protein Therapeutics: Quantitative Analysis I 640-659
Protein Therapeutics: Structural Characterization I 660-678
Proteomics: Clinical Applications 679-712
Proteomics: Quantitative I 713-736
Proteomics: Tissue 737-768
Proteomics: Top Down Analysis I 769-787

TUESDAY POSTERS

Set up all Tuesday posters
7:00 - 8:00 am

Odd-numbered posters present
10:30 - 11:30 am PLUS 12:30 - 2:30 pm

Even-numbered posters present
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Remove all Tuesday posters
7:00 - 8:00 pm

Antibodies & Antibody Drug Conjugates I 001-022
Art, Archaeology & Paleontology 023-036
Biomarkers: Discovery I 037-068
Biomarkers: Quantitative Analysis II 069-099
Clinical Analysis II 100-123
Disease Biomarkers I 124-141
Energy: Hydrocarbon and Petrochemical 142-159
Environmental: General II 160-191
Environmental: Pharmaceuticals and Pesticides 192-212
Food Safety II 213-242
Forensics II 243-269
Fundamentals: Ion Structure/Energetics 270-287
Fundamentals: Ionization Mechanisms 288-297
GC/MS: Instrumentation and Applications I 298-318
H/D Exchange: Protein Structure/Function 319-343
Imaging MS: Method Development I 344-364
Imaging MS: Pharmaceutical Applications 365-379
Imaging MS: Sample Preparation 380-387
Imaging MS: Small Molecules 388-407
Imaging MS: Software 408-415
Informatics: Multiomics Integration 416-440
Instrumentation: Mini/Portable/Fieldable MS 441-457
Instrumentation: New Developments in Ion Detection 458-496
Ion Mobility: Applications I 497-519
Ion Mobility: FAIMS/DMS 520-529
Metabolomics: General I 530-549
Metabolomics: Untargeted Metabolite Profiling 550-568
Phosphopeptides: Quantitative Analysis 569-579
Protein Therapeutics: Quantitative Analysis II 580-605
Protein Therapeutics: Structural Characterization II 606-625
Proteins: PTMs I 626-646
Proteomics: Infectious Diseases 647-657
Proteomics: Intact Proteins 658-666
Proteomics: New Approaches I 667-694
Proteomics: Quantitative II 695-717
Proteomics: Top Down Analysis II 718-737
Small Molecules: Qualitative Analysis 738-756
Systems Biology 757-780

POSTER OVERVIEW



Poster Presentation Schedule
Odd-number posters present: 10:30 am - 11:30 am PLUS 12:30 – 2:30 pm
Even-number posters present: 10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm

WEDNESDAY POSTERS

Set up all Wednesday posters
7:00 - 8:00 am

Odd-numbered posters present
10:30 - 11:30 am PLUS 12:30 - 2:30 pm

Even-numbered posters present
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Remove all Wednesday posters
7:00 - 8:00 pm

Ambient Ionization: Applications I 001-031
Antibodies & Antibody Drug Conjugates II 032-064
Biomarkers: Discovery II 065-095
Biomarkers: Quantitative Analysis III 096-126
Biomolecular Structure Analysis: Chemical Crosslinking and Covalent Labeling II 127-153
Cannabis 154-179
Carbohydrates I 180-205
Clinical Analysis III 206-234
Drug Discovery/DMPK/ADME I 235-254
Food "omics" MS Characterization of Food and Nutritional Supplements 255-275
Food Safety III 276-303
Fundamentals: Photodissociation 304-306
GC/MS: Instrumentation and Applications II 307-329
Glycoproteins I 330-350
Homeland Security 351-360
Imaging MS: Disease Markers I 361-379
Informatics: Algorithms and Statistical Advances II 380-402
Informatics: Metabolomics 403-431
Instrumentation: General 432-452
Instrumentation: New Concepts 453-478
Ion Mobility: Applications II 479-500
LC/MS: Chromatography and Software I 501-517
LC/MS: Sample Preparation I 518-542
Lipids: General 543-564
Metabolomics: Targeted and Quantitative Analysis 565-597
Metabolomics: Untargeted Metabolite Profiling II 598-623
Nucleic Acids and Oligonucleotides I 624-641
Peptides: PTM Identification 642-675
Peptides: Targeted and Quantitative Analysis 676-703
Proteins: Complexes/Non-covalent Interactions I 704-720
Proteomics: Quantitative III 721-744
Small Molecules: Quantitative Analysis 745-769
Toxicology 770-789

THURSDAY POSTERS

Set up all Thursday posters
7:00 - 8:00 am

Odd-numbered posters present
10:30 - 11:30 am PLUS 12:30 - 2:30 pm

Even-numbered posters present
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Remove all Thursday posters
2:30 - 3:00 pm

Ambient Ionization: Applications II 001-032
Ambient Ionization: Fundamentals and Instrumentation 033-059
Carbohydrates II 060-085
Data-Dependent Acquisition 086-092
Data-Independent Acquisition 093-111
Disease Biomarkers II 112-130
Drug Discovery/DMPK/ADME II 131-152
Drug Metabolism: Quantitative Analysis 153-159
Elemental Analysis: ICP/MS 160-175
Elemental Analysis: Isotope Ratio MS 176
Exposomics Methodologies and Research Results 177-181
Food "omics" MS Characterization of Food and Nutritional Supplements II 182-203
Glycoproteins II 204-224
Imaging MS: Disease Markers II 225-242
Imaging MS: Method Development II 243-263
Informatics: General, SRM, and DIA 264-272
Ion Mobility: Applications III 273-294
Ion Mobility: Fundamentals 295-320
Isotope Labeling and Fluxomics Applications 321-331
LC/MS: Chromatography and Software II 332-352
LC/MS: Sample Preparation II 353-377
Lipids: ID and Structural Analysis 378-404
MALDI: Applications 405-417
MALDI: Fundamentals and Instrumentation 418-421
MALDI: Sample Preparation 422-430
Metabolomics: Clinical Applications 431-449
Metabolomics: General II 450-478
Metabolomics: Sample Preparation 479-482
Metabolomics: Untargeted Metabolite Profiling III 483-512
Microorganisms: Identification and Characterization 513-540
Nanomaterials 541-548
Nanoscale and Microfluidic Separations and MS 549-566
Natural Products 567-589
Nucleic Acids and Oligonucleotides II 590-611
Peptides: Fragmentation Mechanisms 612-617
Proteins: Complexes/Non-covalent Interactions II 618-635
Proteins: Conformation Analysis and Structural Biology 636-653
Proteins: General and Membrane 654-673
Proteins: PTMs II 674-697
Proteomics: New Approaches II 698-724
Proteomics: Quantitative IV 725-749
Small Molecules: Quantitative Analysis II 750-777

Set up all Monday posters
7:00 - 8:00 am

Odd-numbered posters present
10:30 - 11:30 am PLUS 12:30 - 2:30 pm

Even-numbered posters present
10:30 am - 12:30 pm PLUS 1:30 - 2:30 pm

Remove all Monday posters
7:00 - 8:00 pm

Biomarkers: Quantitative Analysis I 001-032
Biomolecular Structure Analysis:
Chemical Crosslinking and Covalent Labeling I 033-060
Clinical Analysis I 061-083
Drug Metabolism: Qualitative & High Throughput Analysis 084-098
Drug and Metabolite Analysis: Novel Approaches for Dried Biological Samples 099-103
Energy: Biofuels and Algae 104-113
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Environmental: General I 131-161
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Forensics I 201-229
Fundamentals: Ion Activation/Dissociation 230-255
Fundamentals: Ion Molecule, Ion/Ion, Ion/Electron Interactions 256-263
Fundamentals: Ion Spectroscopy 264-275
Fundamentals: Metal Ion Cationization, Metal-Ligand Interactions, Catalysis 276-282
Fundamentals: Molecular Modeling / Quantum Mechanical Calculations 283-291
H/D Exchange: Hardware, Software and Methodology 292-309
High Mass Accuracy/High Performance MS: Applications and Instrumentation 310-331
Imaging MS: Computational Methods and Analysis 332-342
Imaging MS: Instrumentation 343-359
Informatics: Algorithms and Statistical Advances I 360-382
Informatics: Peptide ID and Quantification 383-422
Informatics: Workflow and Data Management 423-445
Instrumentation: New Developments in Ionization and Sampling I 446-469
Instrumentation: New Developments in Mass Analyzers 470-494
Lipids: Profile Analysis 495-529
Lipids: Targeted and Quantitative Analysis 530-558
Metabolomics: Identification of Unknown Metabolites 559-576
Peptides: Sequence Analysis 577-584
Peptidomics 585-598
Phosphopeptides: Enrichment Methods 599-603
Plant "omics" 604-626
Polymers 627-639
Protein Therapeutics: Quantitative Analysis I 640-659
Protein Therapeutics: Structural Characterization I 660-678
Proteomics: Clinical Applications 679-712
Proteomics: Quantitative I 713-736
Proteomics: Tissue 737-768
Proteomics: Top Down Analysis I 769-787

BIOMARKERS: QUANTITATIVE ANALYSIS I
001-032

MP 001 **Method Development and Validation of 20 Amino Acids in Human Plasma Utilizing UPLC-MS/MS Methodology**; Mackenzie Bentley[1]; Dawn Dufield[1]; Marsha Luna[1]; Kimberly Jackson[1]; Brady Roberts[1]; *[1]KCAS Bioanalytical and Biomarker Services, Shawnee, KS*

MP 002 **Determination of Vitamin A, 25-Hydroxyvitamin D2/D3 and Vitamin E in Human Serum by UPLC-MS/MS**; Liang Sun[1]; Changkun Li[1]; Yueqi Li[1]; Taohong Huang[2]; *[1]Shimadzu (China) Co.,LTD. Beijing Branch, Beijing, China; [2]Shimadzu (China) Co., LTD. Shanghai Branch, Shanghai, China*

MP 003 **Bioanalytical Approaches to Quantify "Free", "Drug-bound" and "Total" Interleukin-8 in Tissue Using Immuno-Capture Liquid Chromatography-Mass Spectrometry**; Yue Zhao[1]; Huidong Gu[1]; Dmitry Ostanin[1]; Kezi Unsal-Kacmaz[1]; Katarzyna Urbanska[1]; Jianing Zeng[1]; Yan Zhang[1]; Renuka Pillutla[1]; *[1]Bristol-Myers Squibb Co., Princeton, NJ*

MP 004 **Quality Assessment of Oocytes for *in vitro* Fertilization Using Target Metabolomics Approach**; Ju Wang[1]; Yan Ren[2]; Wei Zheng[3]; Liang Hu[3]; Siqi Liu[2]; *[1]University of Chinese Academy of Sciences, ShenZhen, China; [2]BGI-Shenzhen, Shenzhen, China; [3]Reproductive and Genetic Hospital of Citic-Xiangya, Changsha, China*

MP 005 **Development of a Reference Measurement Procedure for Intact PTH and Peptides for the Improved Diagnosis, Treatment, and Prevention of CKD-MBD**; Candice Z Ulmer[1]; Hubert W Vesper[2]; *[1]Centers for Disease Control and Prevention, Atlanta, GA; [2]Centers for Disease Control and Prevention, Atlanta, GA*

MP 006 **Novel Highly-Specific ID-UHPLC-MS/MS Method for the Measurement of Steroid Hormones and their Conjugates in Human Serum**; Lumi Duke[1]; Paul H Kim[2]; Julianne Cook Botelho[3]; Candice Ulmer[4]; Hubert W Vesper[4]; *[1]CDC Atlanta, Atlanta, GA; [2]Battelle Memorial Institute, Atlanta, GA; [3]Centers for Disease Control and Prevention, Atlanta, GA; [4]Centers for Disease Control and Prevention, Atlanta, GA*

MP 007 **Systems-Wide Analysis of CD44 Knock-Down by In-Depth Quantitative Proteomics in Different Subtypes of Breast Cancer Cells**; Hyeyoon Kim[1,2]; Jung Hun Lee[1]; Joseph Injae Wang[1]; Han Suk Ryu[2]; Dohyun Han[1]; *[1]Proteomics core facility, Biomedical Research Institute, Seoul National University Hospital, Seoul, South Korea; [2]Department of Pathology, Seoul National University Hospital, Seoul National University College of Medicine, Seoul, South Korea*

MP 008 **In-Depth Determination of Single Amino Acid Variants in CD24+ Subpopulation of Pancreatic Cancer by nano LC-MS/MS**; Jianhui Zhu[1]; Zhijing Tan[1]; Xinpei Yi[2]; Jie Zhang[1]; David M. Lubman[1]; *[1]University of Michigan Medical Center, Ann Arbor, MI; [2]Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing, China*

MP 009 **Rapid Quantitative Analytical Method Development and Validation for Insulin-Like Growth Factor-1 Doping Test Using UPLC-Q-Exactive Orbitrap Mass Spectrometry**; Changmin Sung[1]; Minyoung Kim[1]; Oh-seung Kwon[1]; Hophil Min[1]; *[1]Korea Institute of Science and Technology, Seoul, South Korea*

MP 010 **Fast nano LC Separations for High Throughput Body Fluid Analysis with a TIMS Equipped QTOF and 4D Feature Alignment**; Thomas Kosinski[1]; Scarlet Koch[1]; Christian Meier-Credo[1]; Christoph Gebhardt[1]; Heiner Koch[1]; *[1]Bruker Daltonik GmbH, Bremen, Germany*

MP 011 **Quantification of Human ACTH with 25 pg/mL LLOQ in Plasma by an LC-MS/MS Method**; Baichen Zhang[1]; Tian-Sheng Lu[1]; Jinshui Chen[1]; Guangchun Zhou[1]; Elise



Snider[1]; Matthew Allen[1]; Yong-Xi Li[1]; *[1]Medpace Bioanalytical Laboratories, Cincinnati, OH*

MP 012 **Integrative Proteomics Links CSF Biomarkers to Pathological Networks in the Alzheimer's Disease Brain**; Lenora Higginbotham[1]; Lingyan Ping[1]; Eric B. Dammer[1]; Duc M. Duong[1]; Maotian Zhou[1]; Thomas S Wingo[1]; Erik C.B. Johnson[1]; James J. Lah[1]; Allan I. Levey[1]; Nicholas T. Seyfried[1]; *[1]Emory University, Atlanta, GA*

MP 013 **Catch them Sleeping: Quick and Routine Quantification of Melatonin in Plasma with Ultivo LC/TQ**; Mark Sartain[1]; Aaron Boice[1]; *[1]Agilent Technologies, Santa Clara, CA*

MP 014 **High-Sensitivity and High-Resolution Top-Down LC/MS/MS Analysis of Cardiac Troponin Proteoforms**; Timothy N. Tiambeng[1]; Yanlong Zhu[1]; Yutong Jin[1]; Ziqing Lin[1]; Bifan Chen[1]; Song Jin[1]; Ying Ge[1]; *[1]University of Wisconsin Madison, Madison, WI*

MP 015 **Absolute Quantitation of Non-Human Glycan (Neu5Gc) for Gastric Cancer Screening**; Nari Seo[1,2]; Myung Jin Oh[1,2]; Jaekyoung Ko[1,2]; Yoon Jin Choi[3]; Dong Ho Lee[4]; Hyun Joo An[1,2]; *[1]Chungnam national university, Daejeon, South Korea; [2]Asia-Pacific Glycomics Reference Site, Daejeon, South Korea; [3]Department of Gastroenterology, , Korea University Guro Hospital, Seoul, South Korea; [4]Department of Internal Medicine, Seoul National University Bundang Hospital, Seongnam-si, South Korea*

MP 016 **Analytical Method for Quantifying Long-Term Exposure to Acrylamide, Glycidamide, Ethylene Oxide and Acrylonitrile Using High Performance Liquid Chromatography-Tandem Mass Spectrometry**; Liqun Wang[1]; Carmencita Aurora Gostilean[1]; Tasia Nabors[1]; Chui Y. Tse[1]; Hubert W. Vesper[1]; *[1]Centers for Disease Control and Prevention, Atlanta, Georgia*

MP 017 **Development of a Multiplexed Quantitative Peptide Immunoaffinity LC-MS/MS Assay for the Detection of FFPE Protein Biomarkers**; Carlos A Morales Betanzos[1]; Pamela Whalen[2]; Nagappan Mathialagan[3]; Eric L Powell[2]; Mireia Fernandez Ocana[1]; *[1]Pfizer, Andover, MA; [2]Pfizer WRD, La Jolla, California; [3]Pfizer, Groton, CT*

MP 018 **Optimization and Validation of an LC-MS/MS Method for Peripheral Serotonin as a Pharmacodynamic Biomarker of Treatment with Tryptophan Hydroxylase Inhibitors**; Katelyn Reighard Crizer[1]; François Viel[2]; François Samson Thibault[2]; Michelle Palacios[1]; Stephen A. Wring[1]; *[1]Altavant Sciences, Durham, NC; [2]Syneos Health Clinique, Quebec City, PQ*

MP 019 **Development and Comparison of Two High Throughput LC-MS Methods for the Accurate Quantitation of IGF1 in Human Serum**; Pegah Jalili[1]; Yue Lu[1]; Judy Cao[1]; Uma Sreenivasan[2]; Kevin Ray[1]; *[1]MilliporeSigma, St. Louis, MO; [2]MilliporeSigma, Round Rock, TX*

MP 020 **A Systematic Evaluation of Increasing Laser Shots to Enhance the Information Content of the MALDI Analysis of Biological Fluids**; Senait G. Asmellash[1]; Maxim Tsypin[1]; Krista Meyer[1]; Brandon Touchet[1]; Heinrich Roder[1]; *[1]Biodesix, Boulder, CO*

MP 021 **Reducing the Need for Surrogate Matrix or Surrogate Analyte in Biomarker Assays**; Guille Metzler[1]; Richard King[1]; Carmen Fernandez-Metzler[1]; Susan Crathern[1]; *[1]PharmaCadence Analytical Services, Hatfield, PA*

MP 022 **Mass Spectrometry-Based Quantification of Tau in Human Cerebrospinal Fluid Using a Complementary Tryptic Peptide Standard**; Maotian Zhou[1]; Duc M Duong[2]; Jingting Dai[2]; James J. Lah[2]; Allan I. Levey[2]; Nicholas Seyfried[2]; *[1]Emory University, atlanta, GA; [2]Emory University, Atlanta, GA*

MP 023 **Quantification of Specific Organophosphorous Pesticides, Synthetic Pyrethroids, and 2,4-Dichlorophenoxyacetic Acid by LC-MS/MS**; Dickson Wambua[1]; Isuru Vidanage[1]; William Roman[1]; Antonia M. Calafat[1]; Maria Ospina[1]; *[1]Centers for Disease Control and Prevention, Atlanta, Georgia*

MP 024 **Development of a High-Throughput Top-Down-Proteomic Technology to Study the Associations between Apolipoprotein A-I Proteoforms and HDL Function**; Henrique Dos Santos Seckler[1]; John T Wilkins[1]; Jonathan Scott Rink[2]; Luca Fornelli[3]; Richard D Leduc[1]; Allan D. Sniderman[4]; Colby Shad Thaxton[2]; Donald Lloyd-Jones[2]; Philip D. Compton[1]; Neil L Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]Northwestern University, Chicago, IL; [3]University of Oklahoma, Norman, OK; [4]McGill Centre for Translational Research in Cancer, Segal Cancer Centre / Lady Davis Institute, Jewish General Hospital, Montreal, QC*

MP 025 **An Improved IonStar Proteomics Strategy Outperforms Spectronaut in Reliable Quantitative Analysis of Large Biological Cohorts**; Xue Wang[1]; jun qu[2]; *[1]University at Buffalo, Buffalo, NY; [2]University at Buffalo, SUNY, Buffalo, NY*

MP 026 **Use of Mass Spectrometry to Evaluate the Exposure to di-2-ethylhexyl terephthalate in the U.S. General Population from the NHANES 2015–2016**; Manori Silva[1]; Lee-Yang Wong[1]; Ella Samandar[1]; James L Preau[1]; Lily T Jia[1]; Antonia M. Calafat[1]; *[1]Centers for Disease Control and Prevention, Atlanta, Georgia*

MP 027 **Quantification of Plasma Glucosylsphingosine in Patients with Gaucher Disease Using UPLC-MS/MS**; Haoyue Zhang[1]; Sarah P. Young[1,2]; James Beasley[1]; Patricia Mccaw[1]; Deeksha Bali[1,2]; Priya Kishnani[2]; Ashlee Stiles[1,2]; *[1]Biochemical Genetics Laboratory, Duke University Health System, Durham, NC; [2]Division of Medical Genetics, Department of Pediatrics, Duke University School of Medicine, Durham, NC*

MP 028 **Fully Automated Quantitative Assessment of Methylmalonic Acid on Blood Cards Using Direct Isotope Dilution Mass Spectrometry**; Jeremiah C Jamrom[1]; Logan Miller[1,2]; Scott Faber[1]; John Kern[1]; Matt Pamuku[3]; Skip Kingston[1]; Fred D. Foster[4]; *[1]Duquesne University, Pittsburgh, PA; [2]Shimadzu Scientific Instruments, Inc., Columbia, Maryland; [3]Applied Isotope Technologies, Pittsburgh, PA; [4]Gerstel, Inc., Linthicum, MD*

MP 029 **Advanced Mass Spectrometry Strategies for the Discovery of New Biomarkers in Acute Myeloid Leukemia**; Sibylle Pfammatter[1,2,3]; Eric Bonneil[1,2]; Marie Eve Bordeleau[1,2]; Eric Audemard[1,2]; Louis Theret[1,2]; Isabel Boivin[1,2]; Sebastien Lemieux[1,2,4]; Philippe P. Roux[1,2,5]; Josée Hébert[1,2,6,7]; Guy Sauvageau[1,2,8]; Pierre Thibault[1,2,3]; *[1]The Leucegene project at Institute for Research in Immunology and Cancer, Université de Montréal, Montréal, Québec; [2]Institute for Research in Immunology and Cancer, Université de Montréal, Montréal, Québec; [3]Department of Chemistry, Université de Montréal, Montréal, Québec; [4]Department of Computer Science and Operations Research, Université de Montréal, Montréal, Québec; [5]Department of Pathology and Cell Biology, Université de Montréal, Montréal, Québec; [6]Department of Medicine, Faculty of Medicine, Université de Montréal, Montréal, Québec; [7]Division of Hematology-Oncology and Leukemia Cell Bank of Quebec, Maisonneuve-Rosemont Hospital, Montréal, Québec*

MP 030 **HPLC-MS/MS Method for Measuring 15 Urinary Biomarkers of Exposure to Organophosphate Flame Retardants, Plasticizers, and Pesticides**; Nayana K. Jayatilaka[1]; Paula Restrepo[1]; Zachary Davis[1]; Meghan Vidal[1]; Antonia M. Calafat[1]; Maria Ospina[1]; *[1]Centers for Disease Control and Prevention, Atlanta, GA*

MP 031 **Selected Reaction Monitoring (SRM)-Based Rapid Measurement of GABA in Complex Clinical Samples**; Sigmund J Haidacher[1,2]; Kathleen M Hoch[1,2]; Qinglong Wu[1,2]; Jasmohan S Bajaj[3]; Tor C Savidge[1,2]; Anthony M Haag[1,2];

[1]Baylor College of Medicine, Houston, TX; [2]Texas Children's Hospital, Houston, Texas; [3]Virginia Commonwealth University, Richmond, VA

MP 032 **Short Chain Fatty-Acids Analysis in brain by GC/MS to Determine Effect of Bioactive Food in Mouse Model of Alzheimer's Disease**; Eleazar Rojas Santiago[1]; Tauqeerunnisa Syedaa[2]; Daniel Cuervo-Zanattaa[2]; Claudia Perez Cruz[2]; [1]Agilent Technologies, Mexico, Mexico; [2]CINVESTAV, CDMX, Mexico

BIOMOLECULAR STRUCTURE ANALYSIS: CHEMICAL CROSSLINKING AND COVALENT LABELING I
033-060

MP 033 **Protein Tertiary Structure Prediction Based on Statistical Strategies to Incorporate Cross-Linking/Mass Spectrometry Constraints**; Allan Jhonathan Ramos Ferrari[1]; Guilherme Fahur Bottino[1]; Leandro Martínez[1]; Fabio Cesar Gozzo[1]; [1]University of Campinas, Campinas, Brazil

MP 034 **Development of a Capillary LC Method for Co-Elution of Isomeric Peptide Oxidation Products**; Niloofar Abolhasani Khaje[1]; Joshua S Sharp[1]; [1]University of Mississippi, University, MS

MP 035 **Development of a Fast Photochemical Oxidation of Proteins (FPOP)-Based Protein Folding Study**; Luciano H Di Stefano[1]; Danté T Johnson[1]; Lisa M Jones[1]; [1]University of Maryland Baltimore, Baltimore, MD

MP 036 **Characterization of the IL-7/IL-7Rα Binding Interface in Solution with Docking Guided by Mass Spectrometry-Based Cross-linking and Hydrogen Deuterium Exchange Data**; Mengru Mira Zhang[1]; Guodong Chen[2]; Brett R Beno[2]; Richard Y-C Huang[2]; Jagat Adhikari[1]; Ekaterina Deyanova[2]; Jing Li[2]; Michael Gross[1]; [1]Washington University, St. Louis, MO; [2]Bristol-Myers Squibb, Princeton, NJ

MP 037 **Alpha-Synuclein Oligomers Modelled Using Crosslinking and Discrete Molecular Dynamics Simulations and Validated with Multiple Structural Proteomics Techniques**; Nicholas I Brodie[1,2]; Venkat R. Chirasani[3]; Andrew G. Cairns[4]; Fredrick Almqvist[4]; Evgeniy V. Petrotchenko[5]; Nikolay V. Dokholyan[3]; Christoph H. Borchers[1,2,5,6]; [1]University of Victoria-Genome BC Proteomics Centre, Victoria, BC; [2]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; [3]Departments of Pharmacology, and Biochemistry and Molecular Biology, Pennsylvania State College of Medicine, Hershey, PA; [4]Department of Chemistry, Umeå University, Umeå, Sweden; [5]Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; [6]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC

MP 038 **Observing Gleevec's Drug Engagement in TNBC-AA and TNBC-EA Using In-Cell Fast Photochemical Oxidation of Proteins**; Emily E Chea[1]; Lisa M Jones[2]; [1]University of Maryland, Baltimore, Baltimore; [2]University of Maryland Baltimore, Baltimore, MD

MP 039 **Normalizing Covalent Labeling Reactivity to Obtain Better Constraints for Computational Protein Structure Prediction**; Xiao Pan[1]; Richard W. Vachet[1]; [1]University of Massachusetts, Amherst, MA

MP 040 **MaXLinker: An Innovative "MS3-centric" Proteome-Wide Cross-Link Search Engine with High Sensitivity and Specificity**; Kumar Yugandhar[1,2]; Ting-Yi Wang[1,2]; Alden King-Yung Leung[1,2]; Michael Charles Lanz[2,3]; Ievgen Motorykin[4]; Jin Liang[1,2]; Elnur Elyar Shayhidin[1,2]; Marcus Bustamante Smolka[2,3]; Sheng Zhang[4]; Haiyuan Yu[1,2]; [1]Department of Biological Statistics and Computational Biology, Cornell University, Ithaca, NY; [2]Weill Institute for Cell and Molecular Biology, Cornell University, Ithaca, NY; [3]Department of Molecular Biology and Genetics, Cornell University, Ithaca, NY; [4]Mass Spectrometry and Proteomics Facility, Institute of Biotechnology, Cornell University, Ithaca, NY

MP 041 **High-Resolution Hydroxyl Radical Protein Footprinting Introduction and Workflow**; John Schenkel, Jr.[1]; Janna Kiselar[1,2]; Mark Chance[1,2]; [1]NeoProteomics, Inc., Cleveland, OH; [2]Case Western Reserve University, Cleveland, OH

MP 042 **Design, Synthesis and Application of Novel Sulfoxide-Based, Click-Chemistry Enrichable Cleavable Cross-Linkers for Protein-Protein Interaction Analysis**; Michael Stadlmeier[1]; Leander Runtsch[1]; Martin Wühr[2]; Thomas Carell[1]; [1]LMU Munich, Munich, Germany; [2]Princeton University, Princeton, NJ

MP 043 **The Interactome of Mitochondria in Baker's Yeast: A Snapshot Taken by Cross-Linking Mass Spectrometry**; Andreas Linden[1,2]; Ralf Pflanz[1]; Iwan Parfentev[1]; Bettina Homberg[2]; Markus Deckers[2]; Peter Rehling[2]; Henning Urlaub[2,3]; [1]Max Planck Institute for Biophysical Chemistry, Goettingen, Germany; [2]University Medical Center Goettingen (UMG), Goettingen, Germany; [3]Max Planck Institute for Biophysical Chemistry, Goettingen, Germany

MP 044 **Kojak 2.0: New Features for the Analysis of Cross-Linked Proteins**; Michael R. Hoopmann[1]; Alex Zelter[2]; Michael Riffle[2]; Jimmy K Eng[2]; Trisha N Davis[2]; Robert L Moritz[1]; [1]Institute for Systems Biology, Seattle, WA; [2]University of Washington, Seattle, WA

MP 045 **Systems Structural Biology of the Heart: Impact of Lysine Acetylation on Protein Conformations and Interactions**; Juan Chavez[1]; Matthew A Walker[1]; Arianne Caudal[1]; Bo Zhou[1]; Andrew Keller[1]; Rong Tian[1]; James E. Bruce[1]; [1]University of Washington, Seattle, WA

MP 046 **Structural Interrogation of Phosphorylation-Dependent Proteasome Dynamics Using a Multifaceted Cross-Linking and Targeted Quantitation-Based Approach**; Clinton Yu[1]; Lan Huang[1]; Xiaorong Wang[1]; [1]University of California, Irvine, CA

MP 047 **Determination of the Yield of Copper-Catalyzed Click Reaction on Individual Newly Synthesized Proteins with Azidonorleucine Inside Live Cells**; Chengzhi Cai[1]; Guoting Qin[1]; Rufeng Li[1]; [1]University of Houston, Houston, TX

MP 048 **Tyrosine-Specific Nitration of Influenza Hemagglutinin Proteins by Selective Covalent Labeling and Mass Spectrometry**; Carrie L. Pierce[1]; Jonathan L. Bundy[1]; Jakub Baudys[1]; Tracie L. Williams[1]; Dongxia Wang[1]; Maria I. Solano[1]; John R. Barr[1]; [1]Centers for Disease Control and Prevention, Atlanta, Georgia 30341

MP 049 **Acquisition Mode Characterization for the Quantitative and Qualitative Analysis of Cross-Linked Peptides by Targeted and Untargeted LC-IM-MS**; Hannah Britt[1]; Suniya Khatun[1]; Abubakar Hatimy[1]; Jonathan P Williams[2]; Chris Hughes[2]; Tristan Cragnolini[1]; Nathanael Page[3]; Konstantinos Thalassinos[1]; Johannes PC Vissers[2]; [1]UCL, London, United Kingdom; [2]Waters Corporation, Wilmslow, United Kingdom; [3]LGC Group, Teddington, United Kingdom

MP 050 **Tools for Atomic-Resolution Protein Structure Determination in Cells: CID-Cleavable Photo-Amino Acids and Purification of Crosslinked Peptides of Any Origin**; Bjorn-Erik Wulff[1]; Joshua E. Elias[1]; Pehr Harbury[1]; [1]Stanford University, Stanford, CA

MP 051 **Monitoring the Aggregation-Induced Conformational Conversion of α-Synuclein Protein by Fast Photochemical Oxidation of Proteins (FPOP)**; Prashant N. Jethva[1]; Jing Yan[1]; Eva Illes-Toth[2]; Michael L. Gross[1]; [1]Department of Chemistry, Washington University, St. Louis, MO; [2]School of Biosciences, University of Birmingham, Birmingham, United Kingdom

MP 052 **Next Generation Dual Cleavable Cross-Linking Strategies for High Confidence Identification of Cross-Linked Peptides**; Jayanta Kishor Chakrabarty[1]; Fang Zixiang[1]; Abu Hena M. Kamal[1]; Saiful M. Chowdhury[1]; *[1]University of Texas, Arlington, TX*

MP 053 **Determination of Ligand and pH-Induced Conformational Changes in the Cation-Independent Mannose-6-Phosphate Transferase by Fast Photochemical Oxidation of Proteins**; Sandeep K. Misra[1]; Linda J. Olson[2]; Nancy M. Dahms[3]; Joshua S. Sharp[1]; *[1]University of Mississippi, University, MS; [2]Medical College of Wisconsin, Milwaukee, MI; [3]Medical College of Wisconsin, Milwaukee, WI*

MP 054 **Describing the Interaction XcpU and XcpW from the *Pseudomonas aeruginosa* Type II Secretion Machinery Using Cross Linking – Mass Spectrometry**; Badreddine Douzi[1]; Geneviève Ball[1]; Cristian A Escobar Bravo[2]; Edwin De Pauw[3]; Katrina Forest[2]; Romé Voulhoux[1]; Loic Quinton[3]; *[1]CNRS, Aix-Marseille Université, IMM, Laboratoire de Chimie Bactérienne UMR7283, Marseille, France; [2]Department of Bacteriology, University of Wisconsin-Madison, WI, 53706, USA, Madison, WI; [3]Laboratoire de Spectrométrie de Masse - MolSys Research Unit - Liège Université, Liège, Belgium*

MP 055 **Accelerated Biomolecular Cross-Linking by Contained-Electrospray Ionization for Rapid Detection by Mass Spectrometry**; Benjamin J. Burris[1]; Abraham K. Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH*

MP 056 **Novel Methods for Chemical Crosslinking Based Protein Complex Analysis**; Qun Zhao[1]; Yuxin An[1]; Lili Zhao[2]; Lihua Zhang[2]; Yukui Zhang[2]; *[1]Dalian Institute of Chemical Physics, Chinese Academy of Science, Dalian, China; [2]Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China*

MP 057 **Application of Phenyl-based Columns in Improving the Identification of Inter-crosslinked Peptides**; Zixiang Fang[1]; Yehia Z. Baghdady[1]; Kevin A Schug[1]; Saiful M. Chowdhury[1]; *[1]University of Texas Arlington, Arlington*

MP 058 **Energy Barriers to the Pre-amyloid Structural Change of β-2-microglobulin in the Presence of the Amyloidogenic Variant ΔN6 or Amyloid Inhibitors**; Blaise G. Arden[1]; Richard W. Vachet[1]; *[1]University of Massachusetts, Amherst, MA*

MP 059 **OpenPepXL: Sensitive, Comprehensive Identification and Quantification of Protein-Protein Cross-Links**; Eugen Netz[1]; Tjeerd M.H. Dijkstra[1]; Timo Sachsenberg[2]; Oliver Kohlbacher[1, 2, 3, 4]; *[1]Biomolecular Interactions group, Max Planck Institute for Developmental Biology, Tuebingen, Germany; [2]Applied Bioinformatics group, University of Tuebingen, Tuebingen, Germany; [3]Quantitative Biology Center (QBiC), University of Tuebingen, Tuebingen, Germany; [4]Institute for Translational Bioinformatics, University Hospital Tuebingen, Tuebingen, Germany*

MP 060 **XiView: A common platform for the Downstream Analysis of Crosslinking Mass Spectrometry data**; Martin J Graham[1, 2]; Colin Combe[1, 2]; Lars Kolbowski[3]; Juri Rappsilber[1, 2, 3]; *[1]Wellcome Centre for Cell Biology, Edinburgh, United Kingdom; [2]University of Edinburgh, Edinburgh, United Kingdom; [3]Technische Universität Berlin, Berlin, Germany*

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MP 061 **Reducing the Global Burden of Infectious Diseases through Precision Infection Management (PIM)**; Ian Lewis[1]; Fiona Clement[1]; Deirdre L Church[2]; Ashlee Earl[3]; Yonatan Grad[4]; Christopher Naugler[2]; Sergei Noskov[1]; *[1]University of Calgary, Calgary, AB; [2]Calgary Laboratory Services, Calgary, AB; [3]Broad Institute of MIT and Harvard, Cambridge, MA; [4]Harvard T.H. Chan School of Public Health, Boston, MA*

MP 062 **Interference from Sulfonated Metabolites in the Analysis of β-Lapachone in Clinical Human-Plasma Samples Using Liquid Chromatography-Mass Spectrometry**; Seungil Cho[1]; Bo Kyung Kim[1]; Mi-ri Gwon[1]; Young-ran Yoon[1]; *[1]Kyungpook National University, Daegu, South Korea*

MP 063 **Characterization of an Amphetamine Interference from Gabapentin in an LC-HRMS Confirmation Assay**; Ana Celia Grenier[1]; Teresa Pekol[1]; Dana Schubring[1]; Charlene Johnson[1]; Lawrence J Andrade[1]; Robin Hyland[1]; *[1]Dominion Diagnostics, North Kingstown, RI*

MP 064 **Ambient Mass Spectrometry Immunoassays for the Ultra-Sensitive Biomarker Detection and Tissue Glycan Imaging**; Yu Bai[1]; Shuting Xu[2]; Wen Ma[2]; Huwei Liu[2]; *[1]College of Chemistry, Peking University, Beijing, China; [2]Peking University, Beijing, China*

MP 065 **Dried Blood Spheroids for Stabilizing Acylcarnitines in Micro-liter Blood Samples Stored under Ambient Conditions**; Benji Frey[1]; Deidre E. Damon[1]; Abraham K. Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH*

MP 066 **Quantification of 11-plex LSD Enzyme Activity Using LC-MS/MS**; Ryuichi Mashima[1]; Torayuki Okuyama[1]; Mari Ohira[1]; *[1]National Center for Child Health and Development, Setagaya-Ku, Japan*

MP 067 **A Comparison of Tenofovir Diphosphate and Emtricitabine Triphosphate Concentrations Collected in Whole Blood by a Microsampler or Dried Blood Spot**; Amanda P Schauer[1]; Craig Sykes[1]; Jason R Pirone[1]; Nicole White[1]; Hannah Bryan[1]; Angela DM Kashuba[1]; *[1]University of North Carolina, Chapel Hill, NC*

MP 068 **A Sensitive and Robust HPLC – MS/MS (MRM) Method for the Quantitation of Hepcidin in Human Serum**; Jun Liu[1]; Michael Chen[2]; *[1]University of British Columbia, Vancouver, BC; [2]Island Medical Program, Department of Pathology and Laboratory Medicine, University of British Columbia, Vancouver, BC*

MP 069 **Lipid and Apolipoprotein Changes in Response to Inflammation with Type 2 Diabetes**; Bryan Parks[1]; Zsuzsanna Kuklenyik[2]; John R Barr[2]; *[1]Centers for Disease Control and Prevention, Atlanta, GA; [2]Centers for Disease Control and Prevention, Atlanta, Georgia*

MP 070 **Simultaneous Determination of Eight Antiepileptic Drugs and an Active Metabolite in Human Plasma by LC-MS/MS**; Tian Liu[1]; Raghavendhar R Kotha[1]; Stephanie Zalesak[1]; Jace W Jones[1]; James E Polli[1]; Maureen A Kane[1]; *[1]Department of Pharmaceutical Sciences, University of Maryland School of Pharmacy, Baltimore, MD*

MP 071 **Fully Automated LC-MS/MS Analysis of Anticoagulants Using a Stable Isotope Labelled Internal Standards**; Toshikazu Minohata[1, 2]; Yuki Uno[2]; Sigrid Baumgarten[3]; Stéphane Moreau[3]; Fanny Dayot[1]; Jean-François Hoeffler[1]; *[1]Alsachim SAS, Illkirch, France; [2]Shimadzu Corporation, Kyoto, Japan; [3]Shimadzu Europa GmbH, Duisburg, Germany*

MP 072 **Sensitive Cortisol Analysis Using a Single Hair with Nanoflow UPLC- MS3 Tandem Mass Spectrometry**; Chih-Wei Chang[1, 2]; Linjer Chen[1]; Li-Jung Ma[1]; Pin-Hsuan Wang[1]; Yet-Ran Chen[2]; Pao-Chi Liao[1]; *[1]Department of Occupational and Environmental Health, Medical College, National Cheng Kung University, Tainan, Taiwan; [2]Agriculture Biotechnology Research Center, Academia Sinica, Taipei, Taiwan*

MP 073 **A Two-Minute Liquid Chromatography/Ion Mobility Mass Spectrometry Method for Quantitation of 25-Hydroxyvitamin D without Interference from 3-epi-25-Hydroxyvitamin D**; Nicholas Oranzi[1]; Jiajun Lei[1]; Timothy J. Garrett[1]; Richard A Yost[1]; *[1]University of Florida, Gainesville, FL*

MP 074 **A High-Performance Liquid Chromatography Tandem Mass Spectrometry Method for the Determination of Superwarfarin Rodenticides in Human Plasma**; Daniel Nosal[1]; Douglas L Feinstein[2]; Richard B. van Breemen[3]; *[1]Oregon State University - Linus Pauling Institute, Corvallis, OR; [2]University of Illinois at Chicago, Department of Anesthesiology, Chicago, IL; [3]Linus Pauling Institute, Oregon State University, Corvallis, OR*

MP 075 **Assessing Isolate-Specific Antimicrobial Resistance Patterns of *Klebsiella pneumoniae***; Thomas D. Horvath[1,2]; Sibel Ak[1,2]; Sigmund J. Haidacher[1,2]; Kathleen Hoch[1,2]; Tor C. Savidge[1,2]; Anthony M. Haag[1,2]; *[1]Department of Pathology and Immunology, Baylor College of Medicine, Houston, TX; [2]Microbiome Center, Texas Children's Hospital, Houston, TX*

MP 076 **Mass spectrometry shows limitations of lectin-based approaches to quantify galactose-deficient IgA1 in circulation of IgA nephropathy patients and controls**; Olivier M. Lardinois[1]; Patrick H. Nachman[2]; Jason G. Williams[1]; Leesa J Deierding[1]; *[1]Mass Spectrometry Research and Support Group, National Institute of Environmental Health Sciences (NIEHS), Research Triangle Park, NC; [2]Division of Renal Diseases and Hypertension, University of Minnesota, Minneapolis, MN*

MP 077 **Elucidating Multi-Omic Molecular Signatures of End-Term Preeclampsia and Gestational Diabetes Mellitus**; Melanie T. Odenkirk[1]; Kristin E. Burnum-Johnson[2]; Brandie D. Taylor[3]; Kelly G. Stratton[2]; Marina A. Gritsenko[2]; Lisa M. Bramer[2]; Bobbie-Jo Webb-Robertson[2]; Jennifer Kyle[2]; Kent J. Bloodsworth[2]; Karl K Weitz[2]; Erin S Baker[1]; *[1]Department of Chemistry, North Carolina State University, Raleigh, NC; [2]Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; [3]College of Public Health, Temple University, Philadelphia, PA 19122*

MP 078 **Development of a Quantitative Method for the Measurement of Free Oligosaccharides in Plasma and Urine from Patients with Aspartylglucosaminuria**; Beniam Berhane[1]; Tim Wood[1]; Laura Pollard[1]; *[1]Greenwood Genetic Center, Greenwood, SC*

MP 079 **Discovery of Tumor-Specific Antigens for Leukemia Immunotherapy Using a Novel Proteogenomic Approach**; Sibylle Pfammatter[1]; Eric Bonneil[1]; Joel Lanoix[1]; Krystel Vincent[1]; Chantal Durette[1]; Jean-Philippe Laverdure[1]; Mathieu Courcelles[1]; Marie-Pierre Hardy[1]; Sebastien Lemieux[1]; Claude Perreault[1]; Pierre Thibault[1]; *[1]Université de Montréal, Montréal, Québec*

MP 080 **Pharmacokinetic Interactions of a Red Clover Botanical Dietary Supplement with Drug Metabolism in Peri- and Post-menopausal Women**; Jaewoo Choi[1]; Luying Chen[2,3]; Scott W. Leonard[1]; Suzanne Banuvar[3]; Elena Barengolts[3]; Marlos Viana[3]; Richard B. van Breemen[2,3]; *[1]Linus Pauling Institute, Oregon State University, Corvallis, Oregon; [2]Linus Pauling Institute, College of Pharmacy, Oregon State University, Corvallis, OR; [3]UIC/NIH Center for Botanical Dietary Supplements Research, Chicago, IL*

MP 081 **An Efficient MS Method for Screening 20 Genotypes of Human Papillomavirus**; Yun Zhao[1]; Shanyun Lin[1]; Panhong Liu[1]; Xuehui Tang[1]; Zhe Ren[1]; Yan Ren[1]; Siqi Liu[1]; *[1]BGI-Shenzhen, Shenzhen, China*

MP 082 **Development of Glycosaminoglycan Assays for Mucopolysaccharidoses Using LC-MS/MS**; Takanari Hattori[1]; Tetsuo Iida[1]; Jun Watanabe[1]; Misa Tanaka[2]; Hironori Kobayashi[3]; Shunji Tomatsu[4]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]MS specialite, Yokohama, Japan; [3]Department of Pediatrics, Shimane University Faculty of Medicine, Izumo, Japan; [4]Nemours/Alfred I. duPont Hospital for Children, Wilmington, Delaware*

MP 083 **A Rapid LC-MS/MS Method to Measure Simultaneously IDUA, IDS, NAGLU, GALNS and ASRB Enzymes Activities in Dried Blood Spots**; Misa Tanaka[1]; Jun Watanabe[2]; Tetsuo Iida[2]; Hironori Kobayashi[3]; *[1]MS specialite, Yokohama, Japan; [2]Shimadzu Corporation, Kyoto, Japan; [3]Department of Pediatrics, Shimane University Faculty of Medicine, Izumo, Japan*

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MP 084 **Efficient and Comprehensive Metabolite Identification by Utilizing Automatic Background Exclusion and Specific Filtering Features of Orbitrap ID-X Tribrid Mass Spectrometer**; Kai Wang[1]; Sven Hackbusch[2]; Kate J. Comstock[2]; Kevin Coe[1]; *[1]Janssen R&D, San Diego, CA; [2]Thermo Fisher Scientific, San Jose, CA*

MP 085 **A New Strategy Optimized for Metabolite Profiling on a Tribrid Mass Spectrometer Platform**; Qian Ruan[1]; Kenneth P. Matuszak[2]; Kate J. Comstock[3]; *[1]Bristol-Myers Squibb, Princeton, NJ; [2]ThermoFisher Scientific, Bannockburn, IL; [3]ThermoFisher Scientific, San Jose, CA*

MP 086 **Application of Novel Background Exclusive DDA for Automated and Sensitive MS/MS Acquisition of Unknown Herbal Medicine Components in Biological Samples**; Tingting Cai[1]; Chunyan Zhu[2]; Ying Jin[2]; Jiayun Chen[2]; Guoqiang Liu[3]; Niusheng Xu[3]; Caisheng Wu[2]; Mingshe Zhu[4]; *[1]WuXi AppTec, Nanjing, China; [2]Xiamen University, Xiamen, China; [3]Thermo Fisher Scientific, Shanghai, China; [4]MassDefect Technologies, Princeton, NJ*

MP 087 **Highly Accurate Detection and Identification Methodology of Xenobiotic Metabolites Using Stable Isotope Labeling, LC/HRMS/MS Analysis, and Data Mining Techniques**; Masatomo Takahashi[1]; Yoshihiro Izumi[1]; Fukumatsu Iwahashi[2]; Yasumune Nakayama[3]; Mitsuhiko Iwakoshi[2]; Motonoa Nakao[1]; Seiji Yamato[2]; Eiichiro Fukusaki[4]; Takeshi Bamba[1]; *[1]Medical Institute of Bioregulation, Kyushu University, Fukuoka, Japan; [2]Sumitomo Chemical Co., Ltd., Takarazuka, Japan; [3]Graduate School of Biotechnology and Life Science, Sojo University, Kumamoto, Japan; [4]Graduate School of Engineering, Osaka University, Suita, Japan*

MP 088 **Integrating Discovery-Stage Metabolite Analysis into High-Throughput Microsomal Clearance Pipelines**; Elyse Freiberger[1]; David Wagner[1]; *[1]AbbVie Inc., North Chicago, IL*

MP 089 ***in vitro* Metabolic Studies of SARMs RAD-140 and S-23 in Horse Using Ultra-High Performance Liquid Chromatography–High Resolution Mass Spectrometry**; Yat Ming So[1]; Timmy Lai Sheung Choi[1]; Gary Ngai Wa Leung[1]; Pauly Kit Sze Chan[1]; Ming Yip Lau[1]; Emmie Ngai Man Ho[1]; *[1]Racing Laboratory, The Hong Kong Jockey Club, Hong Kong, Hong Kong*

MP 090 **Investigating Clozapine-Related Protein Binding *in vitro* by LC-MS/MS**; Timon Geib[1]; Lekha Sleno[1]; *[1]UQAM, Montreal, QC*

MP 091 **Involvement of Olmutinib Reactive Metabolites on its Severe Toxic Reactions: Potential Answers by Mass Spectrometry**; Adnan A Kadi[1]; Mohamed W. Attwa[1,2]; Ali S. Abdelhameed[1]; *[1]College of Pharmacy, King Saud University, Riyadh, SA, Riyadh, Saudi Arabia; [2]Students' University Hospital, Mansoura, Egypt*

MP 092 **Balancing Quality and Quantity in Quan/Qual LC-HRMS Analysis**; Anne-Charlotte Dubbelman[1]; Filip Cuyckens[2]; Lieve Dillen[2]; Rob J. Vreeken[1,2]; Thomas Hankemeier[1]; *[1]Leiden University, Leiden, Netherlands; [2]Janssen R&D, Beerse, Belgium*

MP 093 **Metabolism Study of Simvastatin in Rat Tissues Using MALDI Orbitrap Mass Spectrometry**; Wencui Yin[1]; Adnan A Kadi[1]; Alwabli Reem[1]; Rahman M A f m[1]; *[1]King Saud University, Riyadh, Saudi Arabia*

MP 094 **Ultraviolet Photodissociation Enables Confirmation of Site Specific Glucuronidation on Small Molecule Metabolites**; Joe R. Cannon[1]; Zhoupeng Zhang[1]; Joshua Nicklay[2]; Romain Huguet[2]; Scott M. Peterman[2]; Nichoals Duczak[2]; Mark Cancilla[1]; *[1]Merck & Co., Inc., West Point, PA; [2]Thermo Fisher Scientific, San Jose, CA*

MP 095 **Quantitative Analysis of Hair Samples for Methotrexate (MTX) and Metabolite Using High-Performance Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS) Detection**; Yeongsuk Yoo[1]; Sang Kwang Lee[2]; Kun Cho[3]; *[1]Korean Basic Science Institute, Cheong-ju, South Korea; [2]Eulji Medi-Bio research institute, Daejeon, South Korea; [3]Korea Basic Science Institute, Seoul, South Korea*

MP 096 **High Throughput Drug Accumulation Assay and Impact on Metabolome of Drug-Resistant Bacteria**; Vincent Bonifay[1]; Inga V. Leus[2]; Brinda Chandar[2]; Helen I. Zgurskaya[2]; *[1]University of Oklahoma, Norman, OK; [2]University of Oklahoma, Norman, OK*

MP 097 **Improving Peptide Catabolism Interpretation Using Ion Mobility Data and Server-Based Data Review with HELM Integration**; Mark D Wrona[1]; Gordon Murray[2]; Russell Mortishire-Smith[3]; Yun W Alelyunas[1]; Antoni Riera[4]; Tatiana Radchenko[5]; Anna Escola[4]; Ismael Zamora[5]; Jayne Kirk[3]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Beverly, MA; [3]Waters Corporation, Wilmslow, United Kingdom; [4]Institute for Research in Biomedicine (IRB Barcelona), The Barcelona Institute of Science and Technology, Barcelona, Spain; [5]Lead Molecular Design, S.L., Sant Cugat Del Valles, Spain*

MP 098 **El-MAVEN : First in Class Mass Spectrometry Data Processing Engine for Metabolomics**; Shefali Lathwal[1]; Shubhra Agrawal[1]; Raghav Sehgal[1]; Surbhi Poddar[1]; Rishabh Gupta[1]; Saiful Khan[1]; Sahil Kumar[1]; Sabu George[1]; Swetabh Pathak[1]; Abhishek Jha[2]; *[1]Elucidata, Delhi, India; [2]Elucidata, Cambridge, MA*

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MP 099 **Fully Automated Forensic Screening of Dried Bloodspots with MRM Spectrum Mode**; Davor Fielitz[1]; Stefan Gaugler[2]; Jana Rykl[3]; Maha Khalid Almazraoua[4]; Matthias Grill[5]; Vicente L. Cebolla[6]; Asem Quanair[7]; *[1]Shimadzu Deutschland GmbH, Berlin, Germany; [2]CAMAG, Muttenz, Switzerland; [3]Shimadzu Switzerland, Reinach, Switzerland; [4]The Regional Poison Control Center, Dammam, Saudi Arabia; [5]Lipomed, Arlesheim, Switzerland; [6]Instituto de Carboquímica, Zaragoza, Spain; [7]Analytica One, Al-Hidd, Bahrain*

MP 100 **Probing Protein-Ligand Interactions by Native LESA Mass Spectrometry**; Eva Illes-Toth[1]; Helen J. Cooper[1]; *[1]University of Birmingham, Birmingham, United Kingdom*

MP 101 **Incorporating Novel Synthetic DBS Substrates into a Blood Microsampling Device for Multi-Omics Analyses**; Kyle Bachus[1]; Lada Staskova[2,3]; Jeff Craig[3,4]; Robert Shellie[5]; Ricardo Neto[6]; Dario Arrua[6]; Emily F Hilder[6]; Andrew Gooley[1]; Wei Boon Hon[1]; *[1]Trajan Scientific and Medical, Ringwood, Australia; [2]RMIT University, Melbourne, Australia; [3]Centre for Molecular and Medical Research, School of Medicine, Faculty of Health Deakin University, Geelong, Australia; [4]Murdoch Children's Research Institute, The Royal Children's Hospital, Parkville, Australia; [5]Centre for Advanced Sensory Science (CASS), School of Exercise and Nutrition Sciences, Deakin University, Melbourne, Australia; [6]Future Industries Institute, University of South Australia, Mawson Lakes Campus, Adelaide, Australia*

MP 102 **Organic Synthesis Reaction Monitoring of a Fentanyl Synthesis Using a Microporous Polyolefin Silica Substrate for Paper Spray Mass Spectrometry**; Thomas D Kiselak[1]; Imesha W. DeSilva[2]; Anika Claassen[2]; Guido F. Verbeck[2]; *[1]University of North Texas, Roanoke, TX; [2]University of North Texas, Denton, TX*

MP 103 **Enabling Patient Centricity in Clinical Development through at Home Sample Collection**; Melanie Anderson[1]; Daniel Dreyer[1]; Lingling Xue[1]; Marissa Dockendorf[1]; Kevin P. Bateman[1]; *[1]Merck & Co., West Point, PA*

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MP 104 **Application of Thin-Layer Chromatography to Deep Investigation of Maltenes and Asphaltenes Compound Classes by Ultra-High Resolution Mass-Spectrometry**; Alexander Zherebker[1]; Yury kostyukevich[1]; Oleg Kharybin[1]; Gleb Vladimirov[1]; Eugene (evgeny) Nikolaev[1]; *[1]Skolkovo institute of science and technology, Moscow Region, Russian Federation*

MP 105 **Comprehensive Analysis of Isoprenoid Pathway Intermediates and Associated Metabolites by HILIC-QTOF LC/MS**; Edward Baidoo[1]; Yuqin Dai[2]; Veronica Teixeira Benites[1]; *[1]Joint BioEnergy Institute/LBNL, Emeryville, CA; [2]Agilent Technologies, Santa Clara, CA*

MP 106 **Structure Dependent Electrospray Ionization Response ofb-O-4 lignin Compounds**; Shardrack O. Asare[1]; Bert C. Lynn[1]; *[1]University of Kentucky, Lexington, KY*

MP 107 **Insight into Biomass Pyrolysis from Molecular Beam Mass Spectrometry**; Steven M Rowland[1]; Anne K Starace[1]; Kristen Hietala[1]; Daniel L Carpenter[1]; *[1]National Renewable Energy Lab, Golden, CO*

MP 108 **Detailed Chemical Composition of an Oak Biocrude and Its Hydrotreated Product Determined by Positive Atmospheric Pressure Photoionization FT-ICR Mass Spectrometry**; Alan G. Marshall[1]; Rebecca L. Ware[2]; Ryan P. Rodgers[2]; Ofei D Mante[3]; David C Dayton[3]; Sylvain Verdier[4]; Steven M Rowland[2]; *[1]NHMFL, Florida State Univ., Tallahassee, FL; [2]National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; [3], RTI International, Research Triangle Park, NC; [4]Haldor Topsoe A/S, Lyngby, Denmark*

MP 109 **Coupling LC-MS/MS-Based Proteomics and Targeted Metabolite Analysis Reveals Novel Enzymatic Solutions for Lignin Utilization and Valorization in *Novosphingobium aromaticivorans***; Richard J. Giannone[1,2]; David C Garcia[3,4]; Gerald N Presley[2,3]; Jacob H Cecil[3]; Joshua K Michener[2,3]; *[1]Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN; [2]Center for Bioenergy Innovation, Oak Ridge National Laboratory, Oak Ridge, TN; [3]Biosciences Division, Oak Ridge National Laboratory, Oak Ridge, TN; [4]The Bredesen Center for Interdisciplinary Research and Graduate Education, University of Tennessee, Knoxville, TN*

MP 110 **High-Resolution Mass Spectrometry (FT-ICR) Analysis of Milled Wood Lignins**; Evan Terrell[1]; Vincent Carré[2]; Frédéric Aubriet[2]; Anthony Dufour[3]; Manuel Garcia-Perez[1]; *[1]Washington State University, Pullman, WA; [2]Université de Lorraine, ICPM, Metz, France; [3]Université de Lorraine, LRGP, CNRS, Nancy, France*

MP 111 **Application of Gas Chromatography - Mass Spectrometry for the Analysis of Structural Isomers of Lignin Dimers**; Poorya Kamali[1]; Bert C. Lynn[1]; *[1]Department of Chemistry, University of Kentucky, Lexington, KY*

MP 112 **Using SPME-GC-MS for Chemical Profiling of Volatile Organic Compounds Emitted as Early Biomarkers of Algal Pond Crashes**; Kristen L. Reese[1,2]; Carolyn L. Fisher[3]; Matthew W. Moorman[4]; A. Daniel Jones[2]; Matthias Frank[1]; Todd W. Lane[3]; *[1]Lawrence Livermore National Laboratory, Livermore, CA; [2]Michigan State University, East Lansing, MI; [3]Sandia National Laboratory, Livermore, CA; [4]Sandia National Laboratory, Albuquerque, NM*

MP 113 **Data Mining and Machine Learning Strategies for Non-Targeted Interpretation of High-Resolution Mass Spectrometry Data from Complex Biofuel Samples**; Sasa Bjelic; *Paul Scherrer Instut, Villigen PSI, Switzerland*

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MP 114 **Identification of Transformation Products and Disinfection By-Products in Wastewater Impacted Drinking Water**; Danielle C. Westerman[1]; Hannah K Liberatore[1]; Kristin H Cochran[1]; Cassiana Montagner[2]; Michael J Plewa[3]; Leslie H Cizmas[4]; Jeanne VanBriesen[5]; Dionysios Dionysiou[6]; Ying Huang[6]; Daniel Schlenk[7]; Keith Loftin[8]; Tarun Anumol[9]; Susan D. Richardson[1]; *[1]University of South Carolina, Columbia, SC; [2]University of Campinas, Campinas, Brazil; [3]University of Illinois Urbana-Champaign, Urbana-Champaign, IL; [4]Texas A&M University, College Station, TX; [5]Carnegie Mellon University, Pittsburgh, PA; [6]University of Cincinnati, Cincinnati, OH; [7]University of California Riverside, Riverside, CA; [8]U.S. Geological Survey, Lawrence, KS; [9]Agilent Technologies, Wilmington, DE*

MP 115 **Per- and Polyfluoroalkyl Substances (PFAS) Analysis in Human Serum and Plasma by Ultra-Performance Liquid Chromatography - Tandem Mass Spectrometry (UPLC-MS/MS)**; M Abdul Mottaleb[1,2]; Michael Petriello[1,2]; Jennifer Miller[3]; Susan S Smyth[1,2]; Debra K Moser[3]; Andrew J Morris[1,2]; *[1]Division of Cardiovascular Medicine, University of Kentucky, Lexington, KY; [2]Lexington Veterans Affairs Medical Center, Lexington, KY; [3]College of Nursing, University of Kentucky, Lexington, KY*

MP 116 **Determination of Novel Dihydroxylated Polybrominated Diphenyl Ethers in Sea Fish by Gas Chromatography - Tandem Mass Spectrometry**; Mengtao Zhang[1]; Jianghong Shi[2]; Zongwei Cai[1]; *[1]Hong Kong Baptist University, Hong Kong, China; [2]Southern University of Science and Technology, Shenzhen, China*

MP 117 **Discovery of Novel N-(4-hydroxybenzyl)valine Hemoglobin Adducts in Human Blood.**; Amanda Degner[1,2]; Henrik Carlsson[3]; Isabella Karlsson[3]; Johan Eriksson[3]; Andrew Rajczewski[1,2]; Suresh Pujari[1,2]; Margareta Törnqvist[3]; Natalia Tretyakova[1,2]; *[1]University of Minnesota, Minneapolis, MN; [2]Masonic Cancer Center, U of MN, Minneapolis; [3]Stockholm University, Stockholm, Sweden*

MP 118 **Quantification of Persistent Organic Pollutants in Human Blood Using Stir Bar Sorptive Extraction, GC/MS/MS, and Isotope Dilution Mass Spectrometry**; Weier Hao[1]; Ashley Dillard[1]; Anthony Macherone[2]; Jack Stuff[3]; Scott Faber[4]; Skip Kingston[1]; Matt Pamuku[5]; *[1]Duquesne University, Pittsburgh, PA; [2]Agilent Technologies, Inc., Wilmington, DE; [3]Gerstel, Inc., Linthicum, MD; [4]The Children's Institute of Pittsburgh, Pittsburgh, PA; [5]Applied Isotope Technologies, Pittsburgh, PA*

MP 119 **GC-MS-Based Workflow for Discovery and Characterization of Biomarkers of Exposure to Greenness in Human Urine**; Zhengzhi Xie[1]; Rachel Keith[1]; Aruni Bhatnagar[1]; Pawel Lorkiewicz[1]; *[1]University of Louisville, Louisville, KY*

MP 120 **Neutral Loss and Product Ion Filtering to Screen Exposure Biomarkers to Common and Novel Phthalates: Application to a Standards Mixture** ; Syam S. Andra[1]; Georgia Dolios[1]; Divya Pulivarthi[1]; Dhavalkumar Patel[2]; Emily A Spear[3]; Lauren Petrick[1]; Manish Arora[1]; Annemarie Stroustrup[3]; *[1]Department of Environmental Medicine and Public Health, Icahn School of Medicine at Mount Sinai, New York City, NY; [2]School of Pharmacy, Texas Tech University Health Sciences Center, Amarillo, Texas; [3]Department of Pediatrics, Icahn School of Medicine at Mount Sinai, New York City, NY*

MP 121 **IR-MALDESI Mass Spectrometry Imaging of Rat Placenta Tissue after Exposure to Flame Retardants**; Crystal L Pace[1]; Måns Ekelöf[1]; Brian Horman[2]; Heather Patisaul[2,3]; Heather Stapleton[4]; David C Muddiman[1,3,5]; *[1]FTMS Laboratory for Human Health Research, Department of Chemistry, North Carolina State University, Raleigh, NC; [2]Department of Biological Sciences, North Carolina State University, Raleigh, NC; [3]Center for Human Health and the Environment, North Carolina State University, Raleigh, NC; [4]Nicholas School of the Environment, Duke University, Durham, NC; [5]Molecular Education, Technology, and Research Innovation Center (METRIC), North Carolina State University, Raleigh, NC*

MP 122 **A Novel Use of Isotopomers for *in situ* Calibration**; Anthony Qualley[1,2]; Geoffrey Hughes[1,2]; Thomas Malloy IV[3]; Ted Piatkowski[3]; Benjamin A Clapp[2]; H. Mitchell Rubenstein[2]; *[1]UES, Inc., Dayton, OH; [2]USAF-AFRL, WPAFB, OH; [3]Batelle, Columbus, OH*

MP 123 **Characterization of Arsenic Metabolites and Protein-Binding Using Chromatography Coupled to Multiple Mass Spectrometry Techniques**; Hanyong Peng[1]; Bin Hu[2]; Qingqing Liu[1]; Xiufen Lu[1]; Xiaowen Yan[1]; X. Chris Le[3]; *[1]University of Alberta, Edmonton; [2]Wuhan University, Wuhan, China; [3]University of Alberta, Edmonton, AB*

MP 124 ***In vitro* Metabolism of Bisphenol A and Five Analogs by LC-HRMS/MS**; Ons Ousji[1]; Leanne Ohlund[1]; Lekha Sleno[1]; *[1]UQAM, Montreal, QC*

MP 125 **Extractables and Leachables Analysis Using a Quadrupole Time of Flight Mass Spectrometer Using SWATH Acquisition**; Rolf Kern[1]; Patricia Sun[2]; Alex Liu[2]; *[1]SCIEX, Redwood Shores, CA; [2]Sciex, Framingham, MA*

MP 126 **Electrochemical Simulation of Triclosan Metabolism and Toxicological Evaluation**; Hendrik Jan Brouwer[1]; Jean-Pierre Chervet[1]; Linyan Zhu[2]; Stephan Küppers[3]; *[1]Antec Scientific, Zoeterwoude, Netherlands; [2]Maryland Institute for Applied Environmental Health, University of Maryland, 4200 Valley Drive, College Park, MD 20742; [3]Research Center Jülich, Department of Analytics, Jülich, Germany*

MP 127 **Rapid Assessment of Isomeric Diversity in Perfluoroalkyl Substances (PFAS) by Ion Mobility Spectrometry-Mass Spectrometry (IMS-MS)**; James Dodds[1]; John C. Fjeldsted[2]; Erin S Baker[1]; *[1]North Carolina State University, Raleigh, NC; [2]Agilent Technologies, Inc., Santa Clara, CA*

MP 128 **Tracking Microcystin Oxidation Product Formation by Liquid Chromatography/High Resolution Mass Spectrometry (LC/HRMS) and Implications for Process Monitoring and Treatment**; Judy Westrick[1]; Johnna A Birbeck[1]; Nicholas Peraino[1]; David C Szlag[2]; *[1]Wayne State University, Detroit, MI; [2]Oakland University, Rochester, MI*

MP 129 **Detection of Endocrine Disrupting Chemicals (EDCs) and Pharmaceuticals and Personal Care Products (PPCPs) in Environmental Waters Using Online Concentration LC-MS/MS**; Johnna A Birbeck[1]; Judy Westrick[1]; Cassandra L Ward[1]; Diana McKenzie[2]; *[1]Wayne State University, Detroit, MI; [2]Bay Mills Community College, Brimley, MI*

MP 130 **Improving Non-Target Identification of Organic Contaminants by Probabilistic Ranking of Putative Structure Assignments by HR/AM MS(/MS) and Computational Mass Spectrometry**; Gordon Getzinger[1]; P. Lee Ferguson[1]; *[1]Duke University, Durham, NC*

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MP 131 **Polymerization in Place: Decreasing the Mobility of Halogenated Contaminants by Biotic and Abiotic Pathways**; Fan Wang[1]; Shay Frankenfield[1]; Thomas M. Makris[1]; John L. Ferry[1]; *[1]University of South Carolina, Columbia, SC*

MP 132 **Determination of Pharmaceuticals in Wastewater Using Online Extraction by LC-MS/MS**; Bianca Silva[1]; Cesar Augusto Marasco Junior[2]; Paulo Clairmont Feitosa de Lima Gomes[2]; [1]*Unesp, Araraquara, Brazil;* [2]*Unesp, Araraquara, Brazil*

MP 133 **Comprehensive Quantification of 30 Disinfection Byproducts Employing a Gas Chromatograph – Triple Quadrupole Mass Spectrometer (GC-QQQ) from Disinfected Wastewater Effluents**; Susana Y Kimura Hara[1]; Alejandro Ortega-Hernanzdez[1]; [1]*University of Calgary, Calgary, AB*

MP 134 **The PFAS Conundrum: Mass Spectrometry Solutions for Addressing it**; Ruth Marfil-Vega[1]; Brahm Prakash[2]; Gerard Byrne[2]; Tairo Ogura[3]; Yuka Fujito[2]; [1]*Shimadzu Scientific Instruments, Columbia, MD;* [2]*Shimadzu Scientific Instruments, Inc., Columbia, Maryland;* [3]*Shimadzu corp., Kyoto, Japan*

MP 135 **A Comparison of Electrospray Ionization (ESI) and Paper Spray (PS) Ionization for the Analysis of Polyfluoroalkyl Substances (PFAS)**; Tavleen K. Kochar[1]; Megan R. Ogorchock[1]; Gary L. Glish[1]; [1]*University of North Carolina, Chapel Hill, NC*

MP 136 **Investigating Degradation of Fluorinated Compounds in Water Using LC-Plasma Assisted Reaction Chemical Ionization-MS**; Kunyu Zheng[1]; Joseph Lesniewski[1]; Samuel White[1]; Kaveh Jorabchi[1]; [1]*Georgetown University, Washington, DC*

MP 137 **The Removal of Microcystins from Water Using Treated Rice Husk**; Dilrukshika S. W. Palagama[1]; Amila M. Devasurendra[1]; David Baliu-Rodriguez[1]; Jon R. Kirchhoff[1]; Dragan Isailovic[1]; [1]*The University of Toledo, Toledo, OH*

MP 138 **Unraveling Carbon Flow within Microbial Communities Using Stable Isotope Probing Multi-Omic Techniques**; Mary S Lipton[1]; Marina A. Gritsenko[1]; Samuel O. Purvine[1]; Amy A. Boaro[1]; Megan K. Nims[1]; Alexandra Cory[2]; Krystin Riha[1]; Thomas O. Metz[1]; Young-Mo Kim[1]; William C. Nelson[1]; James J. Moran[1]; [1]*Pacific Northwest National Laboratory, Richland, WA;* [2]*Florida State University, Tallahassee, FL*

MP 139 **Analysis of Dioxins Utilizing Time-of-Flight for Low Level Quantitation**; Tim Conjelko[1]; Courtney Milner[1]; Jeff Hollis[1]; Matthew Curtis[1]; [1]*Agilent Technologies, Inc., Santa Clara, CA*

MP 140 **Standard Reference Materials for Measurements of Emerging Contaminants**; Kevin M. Huncik[1]; Jessica L. Reiner[2]; John R. Kucklick[2]; [1]*National Institute of Standards and Technology, Charleston, SC;* [2]*NIST, Charleston, SC*

MP 141 **Mass Spectrometry-Based Investigations of Phytoremediation and Tertiary Water Treatment in the Sewanee Constructed Research Wetland**; Jacqueline N. Langmo[1]; Anthony Wright[1]; Tanisha Ghosh[1]; W. Matthew Henderson[2]; Donovan Godbee[1]; Devon Boullion[1]; Scott Torreano[3]; Deborah Mcgrath[3]; Marsha C. Black[1]; Franklin E. Leach Iii[1]; [1]*University of Georgia, Athens, GA;* [2]*Evironmental Protection Agency, Athens, GA;* [3]*The University of the South, Sewanee, TN*

MP 142 **Legacy and Emerging Perfluorinated Alkyl Substances in Water: Developing an SPE Method for LC-MS/MS Analysis**; Kari Organtini[1]; Kenneth Rosnack[1]; Doug Stevens[1]; Euan Ross[2]; Steven Lai[3]; [1]*Waters Corporation, Milford, MA;* [2]*Waters Corporation, Wilmslow, United Kingdom;* [3]*Waters Corporation, Beverly, MA*

MP 143 **Short Chain Chlorinated Paraffins (SCCPs) Analysis Using Negative Chemical Ionization (CI) and Low Energy EI by High-Resolution GC/Q-TOF**; Sofia Nieto[1]; Matthew Curtis[1]; Nathan Eno[1]; Courtney Milner[1]; Pierre Dumas[2]; [1]*Agilent Technologies, Inc., Santa Clara, CA;* [2]*Institut Nacional de Santé Publique du Québec (INSPQ), Québec, QC*

MP 144 **Analysis of the Wastewater Effluent Samples to Identify Toxic Chemicals Using High-Resolution GC/Q-TOF**; Sofia Nieto[1]; Kai Chen[1]; Courtney Milner[1]; Thomas Young[2]; [1]*Agilent Technologies, Inc., Santa Clara, CA;* [2]*University of California, Davis, Davis, CA*

MP 145 **Direct Analysis of Per- and Polyfluoroalkyl Substances (PFAS) in Ground, Surface and Waste Water by LC-MS/MS**; Cristina C. Jacob[1]; Claudia P.B. Martins[1]; Michael Volny[1]; Alan R. Atkins[2]; Richard F. Jack[3]; [1]*Thermo Fisher Scientific, San Jose, CA;* [2]*Thermo Fisher Scientific, Hemel Hempstead, UK, Hemel Hempstead, United Kingdom;* [3]*Thermo Fisher Scientific, Sunnyvale, California*

MP 146 **Trace Level Determination of Aniline Compounds in Water by Direct Aqueous Injection-UHPLC-MS/MS**; Mingli Zhu[1]; Weifeng Zhang[1]; Lizhong Yang[2]; Xiangdong Zhou[2]; Chengyuan Cai[3]; Feng Qin[4]; [1]*Guangzhou Agricultural Products Quantity and Safety Supervisory Institute, Guangzhou, China;* [2]*PerkinElmer Management(Shanghai) Co.,Ltd., Shanghai, China;* [3]*Perkinelmer Management (Shanghai) Co., Ltd., Shanghai, China;* [4]*PerkinElmer, Inc.,, Woodbridge, ON*

MP 147 **Semi-Automated Cleanup of Persistent Organic Pollutants in Environmental Samples - Complete Separation of PCDD/Fs and PCBs for Extracts in Toluene**; Hamid Shirkhan[1]; Rudolf Addink[1]; [1]*Toxic Report, Watertown, MA*

MP 148 **How is β-Cyclocitral Formed in SPME GC/MS of a Cyanobacterium?**; Ryuji Yamashita[1]; Keisuke Kanei[1]; Eri Yamauchi[1]; Koji Tomita[2]; Kiyomi Tsuji[3]; Ken-ichi Harada[1]; [1]*Meijo University, Nagoya, Japan;* [2]*Aichi Prefectural Institute of Public Health, Nagoya, Japan;* [3]*Kanagawa Prefectural Institute of Public Health, Chigasaki, Japan*

MP 149 **Poisoned Honey and Water: An Investigation into the Detection of Pesticides with a Novel Approach to SPE**; Matthew Diplock[1]; Raquel Gonzalez de Vega[1]; Andrew Minett[2]; Philip Doble[3]; [1]*University of Technology Sydney, Sydney, Australia;* [2]*Eprep Pty Ltd, Mulgrave, Australia;* [3]*University of Technology Sydney, Sydney, Australia*

MP 150 **Analysis of Soil Extracts for Degradation Products of the Insensitive Munition DNAN *via* GC/MS-MS**; Jeffrey Michael McGuire[1]; Mark Haley[1]; Michael Simini[1]; Roman Kuperman[1]; [1]*U.S. Army RDECOM Chemical & Biological Center, Aberdeen Proving Ground, MD*

MP 151 **Consequential Effects of Five Bisphenols Contaminated Microplastic Through Water and Simulated Intestinal Fluids: Implications for Human Health**; Pengfei Wu[1]; Yuanyuan Tang[2]; Hangbiao Jin[3]; Zongwei Cai[1]; [1]*HongKong Baptist University, HongKong, China;* [2]*Southern University of Science and Technology, Shenzhen, China;* [3]*Zhejiang University of Technology, Hangzhou, China*

MP 152 **Device and Application of Real-Time VOCs Analysis in Air Based on ESI Mass Spectrometry**; Jiancheng Yu[1]; Junliang Zhang[1]; Keqi Tang[1]; [1]*Ningbo University, Ningbo, China*

MP 153 **Elucidating the Kinetics of Xanthates Decomposition in Mining Waters by Headspace Gas Chromatography-Mass Spectrometry**; Kingsley Donkor[1]; Adrian Batista[1]; William Primrose[1]; [1]*Thompson Rivers University, Kamloops, BC*

MP 154 **Aromatic Core Structure and Heteroatom Chemical Functionality Drive the Transformation of Petroleum into Water-Soluble Organic Matter**; Sydney F Niles[1,2]; Martha L Chacón-Patiño[1]; Huan Chen[1]; Steven M Rowland[1]; Donald F Smith[1]; Christopher L. Hendrickson[1,2]; Alan G. Marshall[1,2]; Ryan P. Rodgers[1,2]; [1]*National High Magnetic Field Laboratory, Tallahassee, FL;* [2]*Florida State University, Tallahassee, FL*

MP 155 **Development of Analysis and Purification Methods for Monitoring Dioxins in Sanitary Napkins**; Young Sang Kwon[1]; Sung-Gil Choi[1]; Seung-Min Lee[1]; Dong Yeol Lee[2]; Sang Gon Kim[2]; Jong-Su Seo[1]; *[1]Korea Institute of Toxicology, Munsan-eup, Jinju, South Korea; [2]Gyeongnam Oriental Anti-aging Institute, Sancheong-gun, South Korea*

MP 156 **Optimizing Extraction and Ionization Method for High Resolution Mass Spectrometry Analysis of Organic Compound**; Sung June Kim[1]; Sunghwan Kim[1]; *[1]Kyungpook National University, Daegu, South Korea*

MP 157 **Rapid Non-Targeted Screening of Aqueous Environmental Samples Using Auto MS/MS**; Imma Ferrer[1]; Daniel L Sweeney[2]; E. Michael Thurman[1]; Jerry A. Zweigenbaum[3]; *[1]University of Colorado Boulder, Boulder, CO; [2]MathSpec, Inc., Arlington Heights, IL; [3]Agilent Technologies, Wilmington, DE*

MP 158 **Analysis of Perfluorinated Compounds in Drinking and Waste Water Using Sequential/Parallel Automated Solid Phase Extraction Using EPA Method 537.1**; Matthew Falkenstein[1]; Tom Hall[1]; *[1]Fluid Management Systems, Watertown, MA*

MP 159 **Performance Trade-offs to Consider when Implementing the High Efficiency, Small Form Factor Ions Sources**; Christopher M Rattray[1]; Julie Kowalski[2]; *[1]Restek Corporation, Bellefonte, PA; [2]Trace Analytics, Spokane, WA*

MP 160 **Electron Ionization Mass Spectrometry as Detection System for Supercritical Fluid Chromatography to Increase Identification Power of Semi-Volatile Compounds**; Francesca Rigano[1]; Roberta La Tella[1]; Paola Dugo[1,2,3]; Luigi Mondello[1,2,3]; *[1]Chromaleont SrL, Messina, Italy; [2]University of Messina, Messina, Italy; [3]University Campus Bio-Medico of Rome, Rome, Italy*

MP 161 **Analysis and Quantitation of Polyfluorinated Alkyl Substances (PFAS) in EPA Method 537.1 Using High Resolution Accurate Mass Spectrometry**; Brahm Prakash[1]; Christopher Gilles[1]; Evelyn Wang[1]; Jerry Byrne II[1]; Yuka Fujito[1]; William Lipps[2]; *[1]Shimadzu Scientific Instruments, Inc., Columbia, Maryland; [2]Eurofins Eaton Analytical, 750 Royal Oaks Drive, Monrovia, CA*

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MP 162 **Monitoring Histone Methyltransferase Activity in Microalgal Extracts by Calorimetric and Mass Spectrometric Approaches**; Amanda L. Wong[1]; Fabiola Zaragoza[1]; Isabella Aguilar[1]; Anthony T. Iavarone[2]; Gary H. Karpen[3]; James J Pesavento[1]; *[1]Saint Mary's College of California, Moraga, CA; [2]QB3/Chemistry Mass Spectrometry Facility, Berkeley, CA; [3]Lawrence Berkeley Laboratory, Berkeley, CA*

MP 163 **Approaching Translational Proteomics: Accurate Quantification of >200 Histone Modifications at a Rate of 50 Samples Per Hour**; Simone Sidoli[1]; Yekaterina Kori[1]; Mariana Lopes[2]; Zuo-Fei Yuan[1]; Hee Jong Kim[1]; Katarzyna Kulej[1]; Kevin A. Janssen[1]; Laura M. Agosto[1]; Julia P.C. Cunha[2]; Andrew J. Andrews[3]; Benjamin A. Garcia[1]; *[1]University of Pennsylvania, Philadelphia, PA; [2]Instituto Butantan, Sao Paulo, Brazil; [3]Fox Chase Cancer Center, Philadelphia, PA*

MP 164 **Dynamics of Histone H3.3K27me3 in Pluripotency and Differentiation of Embryonic Stem Cells Revealed by Stable Isotope Labeling Mass Spectrometry**; Yekaterina Kori[1]; Simone Sidoli[1]; Zuo-Fei Yuan[2]; Benjamin A. Garcia[1]; *[1]University of Pennsylvania, Philadelphia, PA; [2]University of Pennsylvania, Philadephia, PA*

MP 165 **Combining Bioorthogonal Chemistry and Proteomic Profiling to Study the PTM-Specific Interactome of Linker Histone H1**; Eva Hoellmueller[1,2,3]; Martin Scheffner[1,2]; Andreas Marx[1,3]; Florian Stengel[1,2]; *[1]Konstanz Research School Chemical Biology, Konstanz, Germany; [2]Department of Biology, University of Konstanz, Konstanz, Germany; [3]Department of Chemistry, University of Konstanz, Konstanz, Germany*

MP 166 **Enhanced Detection of 5-methyl-2'-deoxycytidine, 5-hydroxymethyl-2'-deoxycytidine, 5-methylcytidine and 5-hydroxymethylcytidine in Human Urine Using HILIC-MS/MS**; Cheng Guo; *Zhejiang University, Hangzhou, China*

MP 167 **Understanding Epigenome and Proteome Remodeling Caused by Novel Germline Histone H3.3 Mutations during Neurodevelopment**; Khadija D Wilson[1]; Geoffrey P. Dann[1]; Elizabeth J. Bhoj[2]; Hakon H Hakonarson[2]; Benjamin A. Garcia[1]; *[1]University of Pennsylvania, Philadephia, PA; [2]Children's Hospital of Philadelphia, Philadelphia, PA*

MP 168 **Epiproteomic Analysis of Archival Formalin-Fixed Paraffin-Embedded Tumor Tissue for Interrogating Oncogenic Mechanisms in Rare Sarcomas**; Dylan Marchione[1]; Ilyana Ilieva[1]; Benjamin A Garcia[1]; John B Wojcik[1]; *[1]The University of Pennsylvania, Philadelphia, PA*

MP 169 **Epigenetics of Alzheimer's disease: Global Chromatin Profiling for Monitoring Histone Post-Translational Modifications in Induced Pluripotent Stem Cell Models**; James Mullahoo[1]; Shawn Egri[1]; Tak Ko[2]; Katherine C. DeRuff[1]; Deborah Dele-Oni[1]; Xiaodong Lu[1]; Malvina Papanastasiou[1]; Jennie Young[2]; Li-Huei Tsai[2]; Jacob D. Jaffe[1]; *[1]Broad Institute, Cambridge, MA; [2]Massachusetts Institute of Technology, Cambridge, MA*

MP 170 **Inhibition of Kinases Reveals Distant Links between Signaling Pathways and the Histone Code**; Kevin A. Janssen[1]; Laura M. Agosto[1]; Benjamin A. Garcia[1]; *[1]Perelman School of Medicine - University of Pennsylvania, Philadelphia, PA*

MP 171 **Use of Microwave-Assisted Acid Hydrolysis for Analysis of Histone Modifications**; Shekufeh Zareian[1]; Michael J Sweredoski[1]; Annie Moradian[1]; Spiros D Garbis[1]; *[1]Caltech, Pasadena, CA*

MP 172 **Proteomic Profiling of Histone Modification Readers Using Self-assembled Multivalent Photoaffinity Peptide Probes**; Kai Zhang[1]; Guijin Zhai[1]; Xue Bai[1]; Shanshan Tian[1]; *[1]Tianjin Medical University, Tianjin, China*

MP 173 **Investigation into Altered 5-hmdC Levels in Cancer Cells**; Jiekai Yin[1]; Yang Yu[1]; Yinsheng Wang[1]; *[1]University of California, Riverside, Riverside, CA*

MP 174 **Novel UHPLC-MRM-MS Approach Allows for Absolute Quantification of Histone PTMs in as Little as 20 Minutes**; Joseph Cesare[1]; Zuofei Yuan[1]; Steven Zhao[1]; Peder Lund[1]; Josue Baeza[1]; Yekaterina Kori[1]; Simone Sidoli[1]; Hee Jong Kim[1]; Hyoungjoo Lee[1]; Kathryn E. Wellen[1]; Benjamin A. Garcia[1]; *[1]University of Pennsylvania, Philadephia, PA*

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MP 175 **Screening of Pesticide Residues in Food by Using High-Throughput GC-MS/MS System with Fast GC Condition**; Junkei Kou[1]; Kiyotaka Konuma[1]; Kouji Okuda[2]; Kazuaki Murayama[1]; Yoshihisa Ueda[1]; *[1]JEOL Ltd, Akishima, Japan; [2]JEOL USA, Inc., Peabody, MA*

MP 176 **Quantitation of Multi Residues Antibiotics in Milk Using LC-MS/MS**; Chandrasekar Madhappan[1]; Dilip Reddy[1]; Manoj G. Pillai[1]; Jianru Stahl-Zeng[2]; *[1]SCIEX, Gurgaon, India; [2]SCIEX, Darmstadt, Germany*

MP 177 **Screening of Multiclass Illegal Adulterants in Supplements and Spices *via* Extracted Common Ion Chromatograms and Neutral Loss Scan by UHPLC-Q/TOF-MS**; Jisu Hur[1]; Beom-Hee Kim[1]; Ki Jung Paeng[2]; Jongki Hong[1]; *[1]Kyung Hee University, Seoul, South Korea; [2]Yonsei university, wonju, South Korea*

MP 178 **Fast and Simlutaneous LC/MS/MS Analysis for Veterinary Drugs in Meat Combined with STQ method**; Natsuyo Asano[1]; Eishi Imoto[1]; Mami Okamoto[1]; Mikie Shima[2]; Jun Watanabe[1]; *[1]Shimadzu corp., Kyoto, Japan; [2]AiSTI Science Co., Ltd., Wakayama, Japan*

MP 179 **Rapid Authentication of Fish Species Using Peptide Probes Isolated in the ProTrap XG**; Alan A. Doucette[1]; Jessica L. Nickerson[1]; Katie Halliday[1]; Joshua Turner[1]; *[1]Department of Chemistry, Dalhousie University, Halifax, NS*

MP 180 **Supercritical Fluid Chromatography Coupled to Tandem Mass Spectrometry for the Analysis of Pesticide Residues in Dried Spices**; Víctor Cutillas[1]; María Murcia-Morales[1]; María del Mar Gómez-Ramos[1]; Ann-Christin Niehoff[2]; Stephane Moreau[2]; Amadeo R. Fernández-Alba[1]; *[1]European Union Reference Laboratory for Pesticide Residues in Fruits & Vegetables. University of Almeria, Agrifood Campus of International Excellence (ceiA3) Department of Hydrogeology and Analytical Chemistry, Almeria, Spain; [2]Shimadzu Europa GmbH, Duisburg, Germany*

MP 181 **EU Compliant Routine Quantitative Dioxin, Dioxin-Like PCB and Marker PCB Analysis by GC-MS/MS Using an Advanced Electron Ionisation Source**; Dominic Roberts[1]; Alexander Schachtele[2]; Richard Law[3]; Tim Anderson[4]; Adam Ladak[4]; Cristian Cojocariu[3]; *[1]Thermo Fisher Scientific, Runcorn, United Kingdom; [2]European Union Reference Laboratory for Halogenated POPs in feed and food, Freiburg, Germany; [3]Thermo Fisher Scientific, Tudor Road, United Kingdom; [4]Thermo Fisher Scientific, Austin, TX*

MP 182 **Comprehensive Identification of Migrating Compounds from Plastic Food Packaging Materials Using High Resolution Accurate Mass Spectrometry**; María José Gómez Ramos[1]; Anna Bauer[2]; Ana Lozano[2]; Amadeo R. Fernández-Alba[2]; *[1]University of Almeria, Almeria, Spain; [2]University of Almeria, Almeria, Spain*

MP 183 **Developing a Robust LC-MS/MS Method for the Determination of Anionic Polar Pesticides in a Range of Food Stuffs without Derivatization**; Dimple Shah[1]; Benjamine Wuyts[2]; Euan Ross[2]; Simon Hird[2]; Keil Brinster[1]; Kenneth Rosnack[1]; Tammy Hicks[1]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Wilmslow, United Kingdom*

MP 184 **A New Automated Approach for the Determination of Mycotoxins in Cereals Using Online SPE-LC-MS/MS**; Peter Ringeling[1]; Boris Bartolec[1]; Cornelis Tump[1]; Gertjan Merjenburgh[1]; Florian Van der Hoeven[1]; Jamie Foss[2]; *[1]Spark Holland, Emmen, Netherlands; [2]PerkinElmer, Shelton, Connecticut*

MP 185 **Multiresidue Analysis of Pesticides in Turmeric (*Curcuma longa*) Powder by GCMS/MS Using QuEChERS' Extraction Method**; Sunil Singh[1]; Durvesh Sawant[2, 3]; Sanket Anand Chiplunkar[2]; Nitish Suryawanshi[2]; Satyendra Thakur[1]; Prashant Hase[2]; Aseem Wagle[2]; Dheeraj Handique[2]; Jitendra Kelkar[2]; Pratap Rasam[2]; Ajit Datar[2]; *[1]Shimadzu Analytical (India) Pvt. Ltd., New Delhi, India; [2]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India; [3]Ramnarain Ruia College, Mumbai, India*

MP 186 **Determination of Coumarin in Electronic Cigarette Liquids by UHPLC Coupled with Isotope Dilution Tandem Mass Spectrometry**; Jingcun Wu[1]; Erasmus Cudjoe[1]; Xia Geng[2]; Joshua Ye[3]; Feng Qin[1]; *[1]PerkinElmer Inc., Woodbridge, ON; [2]PerkinElmer Management(Shanghai)Co.,Ltd., Shanghai, China; [3]Perkin Elmer Canada, Woodbridge, ON*

MP 187 **Application of a Novel Background Exclusion Data-Dependent Acquisition Method to Retrospective Analysis of Target Pesticides and Unknown Xenobiotics in Food**; Chunyan Zhu[1]; Guo-yin Lai[2]; Ying Jin[1]; Guoqiang Liu[3]; Niusheng Xu[3]; Caisheng Wu[1]; Mingshe Zhu[4]; *[1]Xiamen University, Xiamen, China; [2]Xiamen Customs, Xiamen, China; [3]Thermo Fisher Scientific, Shanghai, China; [4]MassDefect Technologies, Princeton, NJ*

MP 188 **High Throughput Target and Suspect Pesticide Analysis Using a New LC/Q-TOF Screener Software**; Karen E Yannell[1]; Kai Chen[2]; *[1]Agilent Technologies, Santa Clara, CA; [2]Agilent Technologies, Inc., Santa Clara, CA*

MP 189 **Up in Vape: What is in my E-Juice Other than Nicotine, Propylene Glycol, and Glycerin**; Ron Honnold[1]; Matthew Curtis[1]; *[1]Agilent Technologies, Inc., Santa Clara, CA*

MP 190 **Analysis of Patulin in Fruit Juices and Extracts Using Liquid Chromatography Triple Quadrupole Mass Spectrometry**; Claudia P.B. Martins[1]; Cristina C. Jacob[1]; Michael Volny[1]; Mary L. Blackburn[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

MP 191 **A Fast, Sensitive and Comprehensive Assay to Quantify Pesticide Residues in Dietary Supplements Using GC/MS/MS Coupled with QuEChERS Extraction Method**; Aihua Liu[1]; Abhijit Ghosh[1]; Spencer Carter[1]; *[1]Dyad Labs, Salt Lake City, UT*

MP 192 **Quantitative Analysis of Aminoglycoside Veterinary Drugs in Solid Milk Products by LC-MS/MS**; Benjamin L. Oyler[1]; James B. Wittenberg[2]; Christine H. Parker[1]; *[1]FDA, College Park, MD; [2]Alcohol and Tobacco Tax and Trade Bureau, Beltsville, MD*

MP 193 **Decomposition and Species Identification in Salmon by High-Resolution Mass Spectrometry with Multivariate Analysis**; Randy Self[1]; Michael McLendon[1]; Christopher Lock[1]; *[1]U.S. FDA, Bothell, WA*

MP 194 **High Throughput Determination of Multi-Class Toxic Alkaloids in Food by High Performance Liquid Chromatography-Tandem Mass Spectrometry**; Guoying Lai[1]; Lijian Wu[1]; Dunming Xu[1]; Zhigang Zhang[1]; Meiling Lu[2]; *[1]Technique Center of Xiamen Customs, Xiamen, China; [2]Agilent Technologies (China) Limited, Beijing, China*

MP 195 **Development and Validation of a New Sensitive and Rapid UPLC-MS-MS Method to Determine Acrylamide in Coffee**; Yilong Zheng[1]; Zhitian Zhang[1]; Jillian O'connell[1]; Junsuo Li[1]; *[1]Intertek, Champaign, IL*

MP 196 **Characterization of Farmer's Cheese with LC-MS/(MS) for Authenticity Purposes**; Henk W. Gerritsen[1]; Robert Jan A.N. Lamers[2]; Martin Alewijn[1]; Marco H. Blokland[1]; Monique G.E.G. Bremer[1]; Ioana M. Barbu[1]; *[1]RIKILT Wageningen UR, Wageningen, Netherlands; [2]Abundnz B.V., Woerden, Netherlands*

MP 197 **Analysis of Odor Components in Fish by Shimadzu Off-Flavor System**; yong wang[1]; Jun Fan[2]; *[1]Shimadzu (China) Co.,Ltd. Beijing Branch, Beijing, China; [2]Shimadzu (China) Co., Ltd. Shanghai Branch, Shanghai, China*

MP 198 **Off-Flavor System of Shimadzu Analyzes the Odor Components in Edible Oil**; Liu Xiaohua; *Shimadzu (China) Co., Ltd., Guangzhou, China*

MP 199 **Discrimination of Soybean Oil and Olive Oil by Benchtop Linear MALDI-TOF**; Dun Junling; *Shimadzu (China) Co., Ltd., Shanghai, China*

MP 200 **Toxin Profiling in Fish Samples from the Indian Ocean Implicated in Ciguatera-Like Poisoning**; Ann Abraham[1]; Katherine Baltzer[1]; Kathleen El Said[1]; Kyle Andrews[1]; *[1]Division of Seafood Science and Technology, FDA, Dauphin Island, AL*

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MP 201 **A High Profile: Detection and Identification of Synthetically-derived Psychoactive Material through Sorbent-Facilitated Headspace Mass Spectral Analysis and Chemometrics**; Meghan G. Fogerty[1]; Rabi A. Musah[1]; *[1]University at Albany-SUNY, Albany, NY*

MP 202 **Investigation of Early Death-Induced Changes in Rat Brain by SPME-HPLC-HRMS: *in vivo* Versus Post Mortem Comparative Study**; Sofia Lendor[1]; Mariola Olkowicz[1]; Ezel Boyaci[1]; Miao Yu[1]; Mustansir Diwan[2]; Nathaly Reyes-Garcés[1]; German Augusto Gómez Ríos[1]; Clement Hamani[2]; Janusz Pawliszyn[1]; *[1]Department of Chemistry, University of Waterloo, Waterloo, ON; [2]Neuroimaging Research Section, Centre for Addiction and Mental Health, Toronto, ON*

MP 203 **Fast Screening of Explosives by Direct Analysis in Real Time Mass Spectrometry**; Mengliang Zhang[1]; Virginia L Benefield[1]; Jared Frazier[1]; *[1]Middle Tennessee State University, Murfreesboro, TN*

MP 204 **Assessing Peptide Profiling Reproducibility of Single Source Human Head Hair** ; Maria Lawas[1]; Katherine F. Jones[1]; Katelyn E. Mason[2]; Deon S. Anex[2]; Traci L. Carlson[1]; Luisa V. Forger[1]; Brian A. Eckenrode[3]; Bradley Hart[2]; Joseph Donfack[3]; *[1]Counterterrorism and Forensic Science Research Unit, Visiting Scientist Program, Federal Bureau of Investigation Laboratory Division, Quantico, VA; [2]Forensic Science Center, Lawrence Livermore National Laboratory, Livermore, CA; [3]Counterterrorism and Forensic Science Research Unit, Federal Bureau of Investigation Laboratory Division, Quantico, VA*

MP 205 **Analytical Separation of Isomeric U-Series Compounds Using Liquid Chromatography Tandem Mass Spectrometry**; Melissa F. Fogarty[1]; Amanda L.A. Mohr[2]; Francis X. Diamond[3]; Barry K Logan[2, 3]; *[1]Center for Forensic Science Research and Education, Willow Grove, PA; [2]CFSRE, Willow Grove, PA; [3]NMS Labs, Willow Grove, PA*

MP 206 **Liquid Chromatography-High-Resolution Mass Spectrometry for the Determination of Cannabinoids, Cannabinoid-Metabolites, and Amphetamine-Type Stimulants in Human Hair**; Sunjoo Kim[1]; Yongho Shin[1]; Won-gu Choi[1]; Hye Suk Lee[1]; *[1]The Catholic University of Korea, Buchen, South Korea*

MP 207 **Comparing the Efficiencies of Common Extraction Methods For Explosive Residues Off Various Surfaces Using Gas Chromatography/ Mass Spectrometry**; Shannon Lamy[1]; Alyssa Marsico[1]; *[1]University of New Haven, West Haven, CT*

MP 208 **On-Site Identification of Forensic Evidence by Novel Coiled Micro-Extraction Sampling Device for Portable GC/MS Instrumentation**; Zachary E Lawton[1]; Leah Rynearson[2]; Marisa San Antonio[2]; Sara M Davis[2]; Sarah Goda[2]; Meghann McMahon[3]; Pauline Leary[4]; Koby Kizzire[2]; Brooke Kammrath[2]; *[1]PerkinElmer, Shelton, CT; [2]University of New Haven, West Haven, CT; [3]Wisconsin State Police, Milwaukee, WI; [4]Federal Resources, Stevensville, MD*

MP 209 **High Resolution Designer Drug Screening Using a High-Sensitivity Q-TOF Mass Spectrometer and an Extended Tandem Mass Spectrum Library**; Jeff Dahl[1]; Rachel Lieberman[2]; Joseph Kahl[3]; Alex Giachetti[3]; *[1]Shimadzu, Columbia, MD; [2]Shimadzu Scientific Instruments, Inc., Columbia, MD; [3]Miami-Dade Medical Examiner Department, Miami, FL*

MP 210 **Identification of Human Haemoglobin Variants through Advanced Forensic Mass Spectrometry of Blood**; Cameron Heaton[1]; Laura Cole[1]; Richard R McColm[2]; Jason Eyre[3]; Simona Francese[1]; *[1]BMRC, Sheffield Hallam University, Sheffield, United Kingdom; [2]DSTL, Porton Down, Salisbury, United Kingdom; [3]BMS Haemolysis Lab, Haematology Department, Sheffield Teaching Hospital, Sheffield, United Kingdom*

MP 211 **An Automated Ignitable Liquid Analysis Workflow for Forensic Laboratories**; Troy J Ernst[1]; Scott J Campbell[2]; John H Moncur[2]; *[1]Michigan State Police - Grand Rapids Laboratory, Grand Rapids, MI; [2]SpectralWorks Limited, Runcorn, United Kingdom*

MP 212 **Peptide Spectral Libraries for Purified Ricin and Forensically Relevant Castor Seed Extracts**; Isabelle G. O'Bryon[1]; Abigail E. Tucker[1]; Brooke L.D. Kaiser[1]; Eric Merkley[1]; Karen L. Wahl[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

MP 213 **A method for Simultaneous Targeted and Non-Targeted LC-HRMS/MS Drug Screening in Forensic Toxicology**; Jason E Schaff[1]; Preston C Lowe[1]; Madeline A Montgomery[1]; Cynthia L Morris-Kukoski[1]; *[1]FBI Laboratory Chem Unit, Quantico, VA*

MP 214 **Use of Image Quality Scores to Determine Fingerprint Age in MALDI imaging**; Madison L Thomas[1]; Paige Hinners[1]; Young Jin Lee[1]; *[1]Iowa State University, Ames, IA*

MP 215 **Thread Spray Mass Spectrometry for Direct Analysis of Hemoglobin in Whole Blood**; Sierra Jackson[1]; Abraham K. Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH*

MP 216 **Rapid and Quantifiable Screening Method for 64 Drugs in Human Blood by Direct Probe Ionization/Tandem Mass Spectrometry (DPiMS)**; Tasuku Murata[1]; Shinji Funatsu[1]; Koretsugu Ogata[1]; Hitoshi Tsuchihashi[2]; Yumi Hayashi[3, 4]; Kei Zaitsu[2, 4]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Department of Legal Medicine and Bioethics, Nagoya University Graduate School of Medicine, Nagoya, Japan; [3]In Vivo Real-Time Omics Laboratory, Institute for Advanced Research, Nagoya University, Nagoya, Japan; [4]Pathophysiological Laboratory Sciences, Department of Radiological and Medical Laboratory Sciences, Nagoya University Graduate School of Medicine, Nagoya, Japan*

MP 217 **Automated immunoaffinity purification of large peptides followed by LC-MS(/MS) analysis**; Monica Mazzarino[1]; Filippo Martinelli[1]; Marta Senofonte[1]; Xavier de la Torre[1]; Francesco Botrè[1, 2]; *[1]Antidoping laboratory, Rome, Italy; [2]Department of Experimental Medicine, "Sapienza" University of Rome, Rome, Italy*

MP 218 **Use of IRMPD Spectroscopy to Characterize Derivatives of Aldehydes Considered Emerging Explosive Threat Compounds**; Connor J Graca[1]; Luke Metzler[1]; Theodore Corcovilos[1]; Giel Berden[2]; Jonathan Martens[2]; Jos Oomens[2, 3]; Michael Van Stipdonk[1]; *[1]Duquesne University, Pittsburgh, PA; [2]Radboud University Nijmegen, Institute for Molecules and Materials, FELIX Facility, Nijmegen, Netherlands; [3]University of Amsterdam, Amsterdam, Netherlands*

MP 219 **Q-Exactive Parameter Optimization for Maximum Signal Intensity when Using LDTD**; Sarah Demers[1]; Serge Auger[1]; Jean Lacoursière[1]; Pierre Picard[1]; *[1]Phytronix Technologies, Quebec, QC*

MP 220 **Evaluation of Micro Volume Sample Preparation Technology Newly Designed for Forensic Toxicology with High Resolution Accurate Mass Spectrometry**; Eishi Imoto[1]; Yujin Natori[2]; Jun Watanabe[1]; Hitoshi Tsuchihashi[2]; Kei Zaitsu[2]; Ichiro Hirano[1]; *[1]Shimadzu corp., Kyoto, Japan; [2]Department of Legal Medicine & Bioethics, Nagoya University Graduate School of Medicine, Nagoya, Japan*

MP 221 **Counterfeit Medicines Identification: A Comparison of Simplified APCI and EI Based MS Methods**; Sangeeta Tanna[1]; Rachel Armitage[1]; John Ogwu[1]; Graham Lawson[1]; *[1]De Montfort University, Leicester, United Kingdom*

MP 222 **Analysis of Cosmetic Products for Evidentiary Value *via* Paper Spray and Paper Cone Spray Ionization-Mass Spectrometry**; Abigail M. Poehls[1]; Shahnaz Mukta[1]; Christopher C. Mulligan[1]; *[1]Illinois State University, Normal, IL*

MP 223 **Rapid Profiling of Authentic Forensic Evidence via Paper Cone Spray Ionization Employed on Portable MS Instrumentation**; Ashley R. Stelmack[1]; William L. Fatigante[1]; Shahnaz Mukta[1]; Christopher C. Mulligan[2]; *[1]Illinois state university, Normal, IL; [2]Illinois State University, Normal, IL*

MP 224 **The Performance of Nanoparticle-Modified Paper Substrates Employed as Surface Transfer Swabs for Combined SERS and PSI-MS Investigation**; Trevor J. McDaniel[1]; Noah W. McClurg[1]; William L. Fatigante[1]; Jun-Hyun Kim[1]; Jeremy D. Driskell[1]; Christopher Mulligan[2]; *[1]Illinois state university, Normal, IL; [2]Illinois State University, Normal, IL*

MP 225 **Electron Ionization (EI) Fragmentation Studies of Reduced Bipyridyl Herbicides: Towards a Reliable Quantitative Approach for Postmortem Samples**; Carlos González[1]; Marielos Arias[1]; Diego Arias[1]; *[1]Sección de Toxicología, Departamento de Ciencias Forenses, San Joaquin de Flores, Costa Rica*

MP 226 **Chemical Differentiation of CITES-Protected Dalbergia Timber Using DART/QToF and TSP/GC/MS**; Dayue Shang[1]; Pamela Brunswick[1]; Jeffrey Yan[1]; Joy Bruno[1]; Philip Evans[2]; Graham Van Aggelen[1]; Marcus Kim[3]; *[1]Environment and Climate Change Canada, North Vancouver, BC; [2]University of British Columbia, Vancouver, BC; [3]Agilent Technologies, Inc., Wilmington, DE*

MP 227 **Simultaneous Analysis of 260 Pesticides in Human Urine Using Scaled-Down QuEChERS Approach and Tandem Mass Spectrometry**; Yongho Shin[1]; Sunjoo Kim[1]; Won-gu Choi[1]; Hye Suk Lee[1]; *[1]The catholic university of korea, Buchen, South Korea*

MP 228 **Application for Forensic Analysis: Discrimination of Fibers Using Trace Organic Additive and Pyrolyzate Marker**; Chikako Takei[1]; Kenichi Yoshizawa[1]; Shinji Azuma[2]; *[1]BioChromato, Inc., Fujisawa, Japan; [2]BioChromato USA, San Diego, California*

MP 229 **Fragmentation Pathways of α-pyrrolidinophenone Derivative Synthetic Cathinones**; Jay Tyler Davidson[1]; Zachary J. Sasiene[2]; Younis Abiedalla[3]; C. Randall Clark[3]; Glen P. Jackson[1,2]; *[1]Department of Forensic and Investigative Science, West Virginia University, Morgantown, WV; [2]C. Eugene Bennett Department of Chemistry, West Virginia University, Morgantown, West Virginia; [3]Department of Drug Discovery and Development, Harrison School of Pharmacy, Auburn University, Auburn, AL*

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MP 230 **Peptide Sequence Influence on the Differentiation of Valine and Norvaline by Hot Electron Capture Dissociation**; Wendy Zhong[1]; Zhidan Liang[2]; Xiang Yu[3]; *[1]Merck, Rahway, NJ; [2]Amgen Inc., Boston, MA; [3]Merck & Co., West Point, PA*

MP 231 **Analysis of Phenetole in its First Excited State and Ionic Ground State: Effects of the Side Chain**; Niklas Helle[1]; Tassilo Muskat[1]; Jurgen Grotemeyer[1]; *[1]Christian-Albrechts-Univ, Kiel, Germany*

MP 232 **Surface-Induced Dissociation of Protein Complexes in an FT-ICR Mass Spectrometer: Experimental and Simulated Performance**; Dalton Snyder[1,2]; Jing Yan[3]; Vicki Wysocki[1,2]; *[1]The Ohio State University, Columbus, OH; [2]Resource for Native Mass Spectrometry Guided Structural Biology, Columbus, OH; [3]Washington University, St. Louis*

MP 233 **Gas-Phase Dissociation of Imidazolium and Benzimidazolium Cations: Effects of Substituent Identity**; Maleesha De Silva[1]; Amanda Patrick[1]; *[1]Mississippi State University, Starkville, MS*

MP 234 **High Energy Collision-Induced Dissociation of Biological Peptides**; Xinyao Jing[1]; Carolyn J Cassady[1]; *[1]The University of Alabama, Tuscaloosa, AL*

MP 235 **Comparison of Reagent Gas for Charge Transfer Dissociation (CTD) Mass Spectrometry of Peptides and Oligosaccharides**; Zachary J. Sasiene[1]; Praneeth M. Mendis[1]; Glen P. Jackson[1,2]; *[1]C. Eugene Bennett Department of Chemistry, West Virginia University, Morgantown, WV; [2]Department of Forensic and Investigative Science, West Virginia University, Morgantown, WV*

MP 236 **Gas Phase Reactions of Heptamethine Cyanine Dyes Using Femtosecond-Laser-Pulse Induced Photodissociation and Collision-Induced Dissociation**; Elena Mitrofanov[1]; Tassilo Muskat[1]; Jurgen Grotemeyer[1]; *[1]Christian-Albrechts-Univ, Kiel, Germany*

MP 237 **Structural Characterization of Intact Proteins Using Electron Capture Dissociation within an Ion Mobility Enabled TOF**; Jonathan P. Williams[1]; Lindsay J. Morrison[2]; Chris Hughes[3]; Jeffery M. Brown[3]; Joseph S. Beckman[4]; Valery G. Voinov[4]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters Corporation, Beverly, MA; [3]Waters Corporation, Wilmslow, United Kingdom; [4]e-Msion Inc., Corvallis, OR*

MP 238 **A Comparison of Negative Ion Radical-Driven Dissociation and Collision-Induced Dissociation on Acidic Peptides**; Can Cui[1]; Chelsea L. Mcmillen[1]; Carolyn J. Cassady[1]; *[1]The University of Alabama, Tuscaloosa, AL*

MP 239 **Multiple-Stage Tandem Mass Spectrometry of Peptide Radical Ions in the Omnitrap Platform**; Mariangela Kosmopoulou[1]; Dimitris Papanastasiou[1]; Roman Zubarev[2]; *[1]Fasmatech, Athens, Greece; [2]Karolinska Institutet, Stockholm, Sweden*

MP 240 **Oligosaccharides – Suppression of Metal-Salt Induced Adducts Using Electrospray-Ionization and SORI-CID Fragmentation**; Volker Iwan[1]; Tassilo Muskat[1]; Jurgen Grotemeyer[1]; *[1]Christian-Albrechts-Univ, Kiel, Germany*

MP 241 **Formation of Non-Zwitterionic π-Centered Glycylglycyltryptophan Radical Cations during the Gas-Phase Dissociation of Zwitterionic Copper(II)–GXW Complexes: Structural,Mechanistic, and Photodissociation Spectroscopic Inves**; Yinan Li[1]; mengzhu li[1]; Chi Kit Andy Siu[2]; Jonathan Martens[3]; Jos Oomens[3]; Keung Ivan Chu[1]; *[1]Department of Chemistry, The University of Hong Kong, Hong Kong, Hong Kong; [2]Department of Chemistry, City University of Hong Kong, Hong Kong, Hong Kong; [3]FELIX Laboratory, Institute for Molecules and Materials, Nijmegen, Netherlands*

MP 242 **Isomeric α-Carbon– and π–Centered Glycylglycyltryptophan Radical Cations and their Dissociation Product Ions: Structural, Energetic, Mechanistic, and Spectroscopic Investigations**; Mengzhu Li[1]; Yinan Li[1]; Chi Kit Andy Siu[2]; Jonathan Martens[3]; Jos Oomens[3]; Keung Ivan Chu[2]; *[1]Department of Chemistry, The University of Hong Kong, Hong Kong, Hong Kong; [2]Department of Chemistry, City University of Hong Kong, Hong Kong, Hong Kong; [3]FELIX Laboratory, Institute for Molecules and Materials, Nijmegen, Netherlands*

MP 243 **Understanding the Perplexing and Interesting Pathways of Peptoid Fragmentation**; Yadwinder Singh Mann[1]; Yuntao Zhang[1]; Jianhua Ren[1]; *[1]University of the Pacific, Stockton, CA*

MP 244 **Accelerating Ion-Molecule Reactions Using Supplemental RF-Activation in a Linear Ion Trap**; Berwyck L. J. Poad[1]; Reuben S. Young[1]; David L. Marshall[1]; Stephen J Blanksby[1]; *[1]Queensland University of Technology, Brisbane, Australia*

MP 245 **The HDX Approach to Evidence the Stepwise Character of Controlled Enantioselective Reduction of Copper (II) Complexes with Polar Amino-Acids, Application**; Ekaterina Dariy[1]; Annelaure Damont[2]; Denis Lesage[3]; Sandra Alves[3]; Alain Perret[1]; Yves Gimbert[4]; François Fenaille[2]; Jean-Claude Tabet[2,3]; *[1]Génomique métabolique, Genoscope, Institut François Jacob, CEA, CNRS, Univ Evry, Université Paris-Saclay, Evry, France; [2]SPI, LEMM, CEA, INRA, Université Paris Saclay, Gif-sur-Yvette, France;*

[3]CNRS, Institut Parisien de Chimie Moléculaire, Sorbonne Universite, IPCM, Paris, France; [4]Université Grenoble Alpes and CNRS, DCM (UMR 5250), Grenoble, France

MP 246 **Novel Cα-Cβ Cleavage of N-terminal Phenylalanine Residues of Tyrosine-Containing Peptide Radical Cations: Structural, Mechanistic, and Photodissociation Spectroscopic Ivestigations**; Wai Kit Tang[1]; Xiaoyan Mu[2]; Naiping Dong[2]; Jonathan Martens[3]; Daniel Michael Spencer[2]; Mengzhu Li[2]; Jos Oomens[3]; Chi Kit Andy Siu[1]; Ivan K. Chu[4]; *[1]Department of Chemistry, City University of Hong Kong, Hong Kong, Hong Kong; [2]Department of Chemistry, University of Hong Kong, Hong Kong, Hong Kong; [3]FELIX Laboratory, Institute for Molecules and Materials, Nijmegen, Netherlands; [4]University of Hong Kong, Hong Kong, Hong Kong*

MP 247 **Hydrogen Atom Attachment to the Histidine and Tryptophan Containing Peptides in Gas-Phase**; Daiki Asakawa[1]; Hidenori Takahashi[2]; Shinichi Iwamoto[2]; Koichi Tanaka[2]; *[1]AIST, Tsukuba, Japan; [2]Shimadzu corp., Kyoto, Japan*

MP 248 **Trends from >10,000 Assigned Fragment Ions in Native Top-Down Mass Spectrometry**; Ashley Ives[1]; Henrique Seckler[1]; Ryan T Fellers[1]; Luis F. Schachner[2]; Steven Matthew Patrie[1]; Neil L Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]Northwestern University, Evanston, IL*

MP 249 **Charge Carrier and Charge State Effects in Free Radical Initiated Peptide Sequencing (FRIPS)**; Eunju Jang[1]; Gabriela Grigorean[1]; Nicholas B. Borotto[1]; Kristina Hakansson[1]; *[1]University of Michigan, Ann Arbor, MI*

MP 250 **Implementation and Characterization of an RF Ion Funnel-Based Surface-Induced Dissociation (SID) Device on a Q-IM-TOF Platform**; Benjamin J Jones[1, 2]; Alyssa Q. Stiving[1, 2]; Joshua D. Gilbert[1]; Zachary L. VanAernum[1, 2]; Sophie R. Harvey[1, 2]; *[1]The Ohio State University, Columbus, OH; [2]Resource for Native Mass Spectrometry Guided Structural Biology, The Ohio State University, Columbus, OH*

MP 251 **Evidence for Reversible Internal Hydride/Deuteride Transfers from Sodiated Deprotonated Fructose-6-Phosphate and Arginine Complex with Solvated Salt Structure**; Ekaterina Dariy[1]; Sandra Alves[2]; Yves Gimbert[3]; Alain Perret[1]; François Fenaille[4]; Jean-Claude Tabet[2, 4]; *[1]Génomique métabolique, Genoscope, Institut François Jacob, CEA, CNRS, Univ Evry, Université Paris-Saclay, Evry, France; [2]CNRS, Institut Parisien de Chimie Moléculaire, Sorbonne Universite, IPCM, Paris, France; [3]Université Grenoble Alpes and CNRS, DCM (UMR 5250), Grenoble, France; [4]SPI, LEMM, CEA, INRA, Université Paris Saclay, Gif-sur-Yvette, France*

MP 252 **An Orthoester Derivatization Strategy for the Structure Elucidation of Vicinal Diols**; Renzo A Samame[1]; Chengli Zu[1]; Daniel Knueppel[1]; Jeffery Gilbert[1]; *[1]Corteva Agriscience, Indianapolis, IN*

MP 253 **Collision-Induced Dissociation of Proton-Bound Base Pairs of 1-Methylcytosine with N-Methylguanines**; Sang Yun Han[1]; Jeong Ju Park[1]; *[1]Gachon University, Seongnam, South Korea*

MP 254 **Dissociation Studies of Astrobiologically Relevant Nucleobase Anions**; Alexandra A Dobbs[1]; Bryan E Metz[1]; Diego T Novoa[1]; Aaron R Wegener[2]; Callie A Cole[1]; *[1]Fort Lewis College, Durango, CO; [2]Texas A&M University, College Station, TX*

MP 255 **Fragmentation of Deprotonated 7- & 9-Methylguanine in an Astrochemical Context**; Diego T. Novoa[1]; Aaron R. Wegener[1, 2]; Alexandra A. Dobbs[1]; Callie A. Cole[1]; *[1]Fort Lewis College, Durango, CO; [2]Texas A&M University, College Station, TX*

FUNDAMENTALS: ION MOLECULE, ION/ION, ION/ELECTRON INTERACTIONS
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MP 256 **An In-Vitro Study of Aromatic Stacking of Drug Molecules**; Ludovic Muller[1]; Shelley N. Jackson[1]; Amina S. Woods[1]; *[1]NIH/NIDA-IRP, Baltimore, MD*

MP 257 **A Gas-phase Reactivity Study of Distonic Phenylcarbenes**; Erlu Feng[1]; Zaikuan Yu[1]; Jacob Milton[1]; Thinh Hoang[1]; Hilkka Kenttämaa[1]; *[1]Purdue University, West Lafayette, IN*

MP 258 **Surface Interaction of Selected Transition Metals and Semiconductors with H2 Plasma Generated Species**; Joshua Rieger[1]; Kai Kroll[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

MP 259 **Charge Inversion of Protein Cations *via* Gas-Phase Ion/Ion Reactions with Hyaluronic Acid Anions**; Hsi-Chun Chao[1]; Mack Shih[1]; Abdirahman M. Abdillahi[1]; Scott A McLuckey[1]; *[1]Purdue University, West Lafayette, IN*

MP 260 **Extracting Mass Information from Large Biomolecules *via* Ion-Ion Reaction Chemistry**; Abdirahman M Abdillahi[1]; Nan Wang[1]; David J. Foreman[1]; Hsi-Chun Chao[1]; Kenneth W Lee[1]; Scott A McLuckey[1]; *[1]Purdue University, West Lafayette, IN*

MP 261 **Characterization of Activated Ion-Electron Transfer Dissociation (AI-ETD) Reaction Kinetics**; Trenton M Peters-clarke[1]; Benton J Anderson[1]; Jean M Lodge[2]; Dain R Brademan[1]; Kevin L Schauer[2, 3]; Michael S Westphall[2]; Joshua J Coon[1, 2, 4, 5]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706; [2]Genome Center of Wisconsin, Madison, WI; [3]Thermo Fisher Scientific, West Palm Beach, FL; [4]Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; [5]Morgridge Institute for Research, Madison, WI*

MP 262 **Gas-phase Photodissociative Crosslinking of Diazirine-Modified Adrenaline with the Binding Motif of beta-2 Adrenergic Receptor**; Yang Liu[1]; Shu R. Huang[1]; Frantisek Turecek[1]; *[1]University of Washington, Seattle, WA*

MP 263 **Thermochemistry of the Ion-Molecule Reactions of Uranium Fluoride Species by Guided Ion Beam Tandem Mass Spectrometry**; Amanda Bubas[1]; Cameron J. Owen[1]; Peter B. Armentrout[1]; *[1]University of Utah, Salt Lake City, UT*

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MP 264 **Investigating Conformational Effects of DNA-drug Interactions by Gas-phase Förster Resonance Energy Transfer**; JoAnn C Chen[1]; Stephen V Sciuto[1]; Rebecca A Jockusch[1]; *[1]University of Toronto, Toronto, ON*

MP 265 **Utility of Infrared Photodissociation Spectroscopy on Identifying Post-Translational Modifications**; Laura Bailey[1]; Larry F. Tesler[1]; Nicolas C. Polfer[1]; *[1]University of Florida, Gainesville, FL*

MP 266 **Nucleophilic Substitution in the Gas Phase by an Unlikely Nucleophile, Cl-, following Anion Attachment**; Gabriel Gaiffe[1, 2]; Maxime C. Bridoux[2]; Jane S. Murray[3]; Peter Politzer[3]; Philippe Maître[4]; Richard B. Cole[1]; *[1]Sorbonne Université, Faculté des Sciences et Ingénierie, Paris, France; [2]Commissariat à l'Energie Atomique - DAM, Bruyères-le-Châtel, France; [3]University of New Orleans, Department of Chemistry, New Orleans, Louisiana; [4]Université Paris-Sud, Laboratoire de Chimie Physique, Orsay, France*

MP 267 **Combining Ultrahigh-Resolution Ion-Mobility Spectrometry with Cryogenic IR Spectroscopy for the Analysis of Glycan Mixtures**; Ahmed Faleh[1]; Stephan Warnke[1]; Thomas R. Rizzo[1]; *[1]EPFL, Lausanne, Switzerland*

MP 268 **An IRMPD Spectroscopic and Computational Study of Gaseous Protonated and Metal Cationized Guanine-Cytosine Base Pairs and Guanine-Containing Mismatches**; Ruodi Cheng[1]; Jonathan Martens[2];

Estelle Loire[3]; Travis Fridgen[4]; [1]*Memorial University of Newfoundland, ST JOHN'S, NL;* [2]*Radboud University Nijmegen, Institute for Molecules and Materials, FELIX Facility, Nijmegen, Netherlands;* [3]*Universite Paris Sud, Orsay, France;* [4]*Memorial University of Newfoundland, St. John's, NL*

MP 269 **Shining Light on Gas-Phase Ions to Study Solvent Effects: Spectral Switching in a Model Dye**; Iden Djavani-Tabrizi[1]; Rebecca A Jockusch[1]; [1]*Department of Chemistry, University of Toronto, Toronto, ON*

MP 270 **Automated UV Action Spectroscopy on a Modified 3D Ion Trap MS for Structural Analysis of DNA Cation-Radicals**; Andy Dang[1]; James Gladden[1]; Yue Liu[1]; Brandon Mozzone[1]; Frantisek Turecek[1]; [1]*University of Washington, Seattle, WA*

MP 271 **Proton and Radical Transfers in Hydrogen-Rich DNA Tetranucleotide Cation Radicals: An Experimental and Computational Study**; Yue Liu[1]; Shu R Huang[1]; Yang Liu[1]; Frantisek Turecek[1]; [1]*University of Washington, Seattle, WA*

MP 272 **Measurement of the Asymmetric UO22+ Stretching Frequency for [UVIO2(X)3]- (X = F, Cl, Br and I) Species Using IRMPD Spectroscopy**; Irena Tatosian[1]; Luke Metzler[1]; Connor J Graca[1]; Theodore Corcovilos[1]; Jonathan Martens[2]; Giel Berden[2]; Jos Oomens[2]; Michael Van Stipdonk[1]; [1]*Duquesne University, Pittsburgh, PA;* [2]*Radboud University Nijmegen, Institute for Molecules and Materials, FELIX Facility, Nijmegen, Netherlands*

MP 273 **Raman Spectroscopy of Solutes in Nano-electrospray Ionization (nESI) Spray Plumes and Neutral Droplets**; Brett Michael Marsh[1]; Denilson de Oliveira[1]; Kiran Iyer[1]; Grace Olivia Capek[1]; Dor Ben-Amotz[1]; R. Graham Cooks[1]; [1]*Purdue University, West Lafayette, IN*

MP 274 **The Insecticide Imidacloprid and some its Fragmentation Products: An IRMPD Spectroscopic and Computational Study**; Kelsey J Menard[1]; Jonathan Martens[2]; Travis Fridgen[1]; [1]*Memorial University of Newfoundland, St. John's, NL;* [2]*FELIX Laboratory, Institute for Molecules and Materials, Nijmegen, Netherlands*

MP 275 **Characterizing Single-TurnAlpha Helices via Cold Ion Spectroscopy of Model Compounds**; John Lawler[1]; Tim Hill[2]; David Fairlie[2]; Scott A McLuckey[1]; Timothy S. Zwier[1]; [1]*Purdue University, West Lafayette, IN;* [2]*University of Queensland, St. Lucia, Australia*

FUNDAMENTALS: METAL ION CATIONIZATION, METAL-LIGAND INTERACTIONS, CATALYSIS
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MP 276 **Detection of Key Reaction Intermediates in Cobalt-Catalyzed Electrochemical CO2 Reduction Using Electrochemical Mass Spectrometry**; Hetong Qi[1,2]; Katherine Walker[3]; Qi Wang[4]; Brian Hivick[2]; Yi Cai[2]; Richard N Zare[3]; Hao Chen[4]; [1]*Xi'an Jiaotong University, Xi'an, China;* [2]*Ohio University, Athens, OH;* [3]*Stanford University, Stanford, CA;* [4]*New Jersey Institute of Technology, Newark, NJ*

MP 277 **Investigation of the C-H Activation Reactivity of Graphene-Supported Single-Atom Catalyst Models in the Gas Phase**; Michael Borrome[1]; Scott Gronert[1,2]; [1]*Virginia Commonwealth University, Richmond, VA;* [2]*University of Wisconsin-Milwaukee, Milwaukee, WI 53211*

MP 278 **Mechanistic Study of C-H Activation of Alcohols and Ethers by a Cationic Iridium(III) Dichloride Phenanthroline Complex**; Rozalie Corea[1]; Scott Gronert[1,2]; [1]*Virginia Commonwealth University, Richmond, VA;* [2]*University of Wisconsin-Milwaukee, Milwaukee, WI*

MP 279 **Using the Phenanthroline as the Chelator to Develop a Method for Fast-Screening of Metal Ions by ESI Mass Spectrometry**; Pai-Chi Syue[1]; Kuok-Fai Li[1]; Bo-Yi Zhang[1]; Hui-Ling Chiang[1]; Ching-yi Lien[1]; Kuo-Lung Ku[1]; [1]*National Chiayi University, Chiayi City, Taiwan*

MP 280 **Utilization of Gas-Phase Tranistion Metal Oxide Complexes LMO+ in Oxidation of Organic Compounds**; Nikko Sideris[1]; Richard a. j. O'hair[2]; Victor Ryzhov[1]; [1]*Northern Illinois University, Dekalb, IL;* [2]*University of Melbourne, Melbourne, Australia*

MP 281 **Decarboxylative Coupling Reactions Catalyzed by First-Row Transition Metal Complexes with Crown Ether**; Elettra L. Piacentino[1]; Fotis Pappas Pappas[2]; Kostantinos Pappas[2]; Michael Lesslie[2]; Thomas M. Gilbert[2]; Richard A. J. O'hair[3]; Victor Ryzhov[2]; [1]*Northern Illinois University, Dekalb;* [2]*Northern Illinois University, Dekalb, IL;* [3]*University of Melbourne, Melbourne, Australia*

MP 282 **Gas-Phase Study of C-N Coupling Reactions Catlayzed by Transition Metal Complexes**; Kevin E Parker[1]; Victor Ryzhov[2]; [1]*Northern Illinois University, DeKalb, IL;* [2]*Northern Illinois University, Dekalb, IL*

FUNDAMENTALS: MOLECULAR MODELING/QUANTUM MECHANICAL CALCULATIONS
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MP 283 **Comparing Theoretical and Experimental Collisional Cross Sections of Carbohydrates to Determine Density Functional Theory Calculation Accuracy**; Emily D. Ziperman[1]; Emvia I. Calixte[1]; Meg E. McCutcheon[1]; Srinivas Pulipaka[1]; Elyssia S. Gallagher[1]; [1]*Baylor University, Waco, TX*

MP 284 **Quasi-Harmonic Approximation for the Thermochemical Stability of Small Proton Bound Clusters – A Theoretical Study**; Alexander Haack[1]; Walter Wissdorf[1]; Hendrik Kersten[1]; Thorsten Benter[1]; [1]*University of Wuppertal, Wuppertal, Germany*

MP 285 **A Novel Concept of Ionisation Site Induced Fragmentation in Positive Ion ESI of C-O Bonds of Ether or Ester Groups**; Maria Ashe[1]; Mansoor Saeed[2]; Peter Howe[2]; Chris K. Skylaris[1]; G. John Langley[1]; [1]*The University of Southampton, Southampton, United Kingdom;* [2]*Syngenta Jealott's Hill International Research Centre, Bracknell, United Kingdom*

MP 286 **Transfer of FeIII from Catechol to Enterobactin Complexes: an Empirical and Theoretical Study**; Daryl Giblin[1]; Lindsey Steinberg[2]; Jan R Crowley[2]; Michael L. Gross[3]; Jeffrey P Henderson[2]; [1]*Washington University, St Louis, MO;* [2]*Washington University, School of Medicine, St. Louis, MO;* [3]*Washington University, St. Louis, MO*

MP 287 **Enhanced Protonation of Amino Acids and Dipeptides Using Cr(III): Developing the Basis for Proteomics Studies**; Rudradatt Persaud[1]; Carolyn J Cassady[1]; David A. Dixon[1]; [1]*The University of Alabama, Tuscaloosa, AL*

MP 288 **Computational Prediction of Gas-Phase Acidities for Small Acidic Peptides and their Amides**; Ashley S McNeill[1]; Can Cui[1]; Justin M Adam[1]; William C Jackson[1]; Michael A Raddatz[1]; Carolyn J Cassady[1]; David A Dixon[1]; [1]*The University of Alabama, Tuscaloosa, AL*

MP 289 **M06-2X and G3(MP2) Proton Affinity Estimation for Organo-Phosphorus Compounds**; Howard G Mayes[1]; Jordan M Rabus[1]; Benjamin J Bythell[1]; [1]*University of Missouri, St. Louis, MO*

MP 290 **MD Simulations on Gaseous Protein Ions Using Solution Force Fields: Is there a Problem?**; Justin H Lee[1]; Lars Konermann[2]; [1]*University of Western Ontario, London, ON;* [2]*University of Western Ontario, London , ON*

MP 291 **Supercharging Mechanism for Unfolded Proteins: Insights from MD Simulations and IMS/MS**; Insa Peters[1]; Haidy Metwally[1]; Lars Konermann[2]; [1]*University of Western Ontario, London , ON ;* [2]*Univ. of Western Ontario, London, ON*

H/D EXCHANGE: HARDWARE, SOFTWARE AND METHODOLOGY
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MP 292 **Thin Film Dialysis HX-MS Reveals Protein Interfaces during Reversible Self-Association of Monoclonal Antibodies at High Concentration**; Mihiri Weerasinghe[1]; Yangjie Wei[2]; Reza Esfandiary[3]; C. Russell Middaugh[2]; David D Weis[1,4]; *[1]1Department of Chemistry, University of Kansas, Lawrence, Kansas (KS); [2]Department of Pharmaceutical Chemistry, University of Kansas, Lawrence, KS; [3]Department of Formulation Sciences, MedImmune LLC, Gaithersburg, MD; [4]2Department of Pharmaceutical Chemistry, University of Kansas, Lawrence, KS*

MP 293 **Which Spectra Should We Pick? Limitations of the Extracted Ion Chromatogram in HDX-LC-MS Analysis**; Jeff Morrow; *Sierra Analytics, Modesto, CA*

MP 294 **A Comparison between Two Automated HDXMS Systems, as Applied to Epitope Mapping**; Aik Roy Heng[1]; Deepa Balasubramaniam[1]; Jonathan Fitchett[1]; Ruben Haro[2]; Michael J. Chalmers[3]; *[1]Lilly Biotechnology Center, San Diego, CA; [2]Discovery Automation, Centro de Investigación, Alcobendas, Spain; [3]Lilly Research Laboratories, Eli Lilly and Company, Indianapolis, IN*

MP 295 **An Algorithm forCalculation of the Protein Fraction Synthetic Rate Using 2 Time Points**; Sergei Ilchenko[1]; Andrew Haddad[1]; Kwangwon Lee[1]; Probodh Sadana[1]; Rovshan Sadygov[2]; Takhar Kasumov[1]; *[1]Northeast Ohio Medical University, Rootstown, OH; [2]University of Texas Medical branch, Galverston, TX*

MP 296 **Single-Residue Resolution of HX-MS Obtained Using ExD in a Q-ToF**; Joseph C. Meeuwsen[1,2]; Yury V. Vasil'ev[1,2]; Valery G. Voinov[1,2]; Nathan I. Lopez[1,2]; Joseph S. Beckman[1,2]; *[1]e-MSion, Inc., Corvallis, OR; [2]Oregon State University, Corvallis, OR*

MP 297 **Sparse Representation for Hydrogen Exchange Mass Spectrometry (HX-MS) Data Using LASSO Optimization**; Yuqi Shi[1]; Jarod Hart[1]; David D Weis[1]; *[1]University of Kansas, Lawrence, KS*

MP 298 **HDX-MS as a Tool for Probing Conformational Stability in Industrial Applications**; Daniel W Pedersen[1,2]; Jeppe C Mouritsen[1]; Christian I Jørgensen[1]; Thomas J D Jørgensen[2]; *[1]Novozymes A/S, Bagsværd, Denmark; [2]University of Southern Denmark, Odense, Denmark*

MP 299 **Optimization of a Low-temperature LC-MS system for Hydrogen/Deuterium Exchange Mass Spectrometry**; Mulin Fang[1]; Zhe Wang[1]; Jiwon Kang[1]; Kellye A Cupp-Sutton[1]; Christina Bourne[1]; Si Wu[1]; *[1]University of Oklahoma, Norman*

MP 300 **Integrated Software Platform for Analyzing Hydrogen-Deuterium Exchange and Oxidative Footprinting Data for Solvent Accessibility**; Wilfred Tang[1]; Marshall Bern[1]; Rose D Lawler[1]; Yong J. Kil[1]; Eric Carlson[1]; Saketh Chemuru[2]; Nicole D Wagner[2]; Liuqing Shi[2]; Henry Rohrs[2]; Daisy W. Leung[2]; Michael L Gross[2]; *[1]Protein Metrics Inc., Cupertino, CA; [2]Washington University, St.louis, MO*

MP 301 **An Integrated, Dual-Proteolysis, -30 oC HPLC Platform for Hydrogen-Deuterium Exchange Mass Spectrometry with Minimized H for D Back-exchange**; Jeffrey W Hudgens[1,2]; Kyle W. Anderson[1,2]; Ioannis Karageorgos[1,2]; *[1]National Institute of Standards and Technology, Rockville, MD; [2]Institute for Bioscience and Biotechnology Research, Rockville, MD*

MP 302 **Refinement of an Algorithm for High-Resolution HDX-MS Data Analysis Combined with HaDeX**; Dominik Cysewski[1]; Weronika Puchala[1]; Aleksandra Badaczewska-Dawid[1]; Katarzyna Dabrowska[1]; Michal Kistowski[1]; Michal Burdukiewicz[2]; Michal Dadlez[1]; *[1]Institute of Biochemistry and Biophysics, Polish Academy of Sciences, Warsaw, Poland; [2]Warsaw University of Technology, Warsaw, Poland*

MP 303 **deMix: Automated HDX-MS Data Analysis Reveals Conformational Isomer Proteins**; Seungjin Na[1]; Jae-Jin Lee[2]; Jong Wha J. Joo[3]; Kong-Joo Lee[2]; Eunok Paek[1]; *[1]Hanyang University, Seoul, South Korea; [2]Ewha Womans University, Seoul, South Korea; [3]Dongguk University-Seoul, Seoul, South Korea*

MP 304 **Characterization of Conformational Differences between Coexisting Protein States Using Differential Hydrogen/Deuterium Exchange during Proteoform Separation**; Yue Shen[1]; Xiuxiu Zhao[1]; Guanbo Wang[1]; David D. Y. Chen[2]; *[1]Nanjing Normal University, Nanjing, China; [2]University of British Columbia, Vancouver, BC*

MP 305 **SelexION® Differential Mobility Hardware Enables Facile, Tunable Gas-Phase Hydrogen-Deuterium Exchange for Small Molecules and Proteins**; Brendon Seale[1,2]; Yves Le blanc[2]; *[1]York University, Toronto, ON; [2]SCIEX, Concord, ON*

MP 306 **Can Spray Solvent Conductivity Modify the Exchange Time for In-Electrospray H/D Exchange of Carbohydrate-Metal Adducts?**; Tara Liyanage[1]; Alexis N. Edwards[1]; Elyssia S. Gallagher[1]; *[1]Baylor University, Waco, TX*

MP 307 **Characterization of Intra-Column Processes in Cross-Path Reactive Chromatography (XP-RC) Using Hydrogen/Deuterium Exchange and MS Detection**; Miaowei Xu[1]; Cedric E. Bobst[1]; Igor A. Kaltashov[1]; *[1]University of Massachusetts, Amherst, MA*

MP 308 **Hydrogen/Deuterium Exchange Coupled to MS/MS to Elucidate Site-Specific Labeling of Carbohydrates**; H. Jamie Kim[1]; Elyssia S. Gallagher[2]; *[1]Baylor University, Waco, TX; [2]Baylor Univeristy, Waco, TX*

MP 309 **20S Proteasome Complex Structure Conformation and Dynamics Study by Hydrogen Deuterium Exchange Mass Spectrometry**; Shaunak Paval[1]; Terry Zhang[2]; Rosa Viner[3]; Albert Konijnenberg[4]; David C Schriemer[1]; Andreas Huhmer[3]; *[1]University of Calgary, Calgary, AB; [2]ThermoFisher, San Jose, CA; [3]Thermo Fisher Scientific, San Jose, CA; [4]Thermo Fisher Scientific, Eindhoven, Netherlands*

HIGH MASS ACCURACY/HIGH PERFORMANCE MS: APPLICATIONS AND INSTRUMENTATION
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MP 310 **New Developments in the Modeling of Ion Fragmentation by MS Interpreter Software**; Alexey V. Mayorov[1]; Yuri A. Mirokhin[1]; Dmitrii V. Tchekhovskoi[1]; Stephen E. Stein[1]; *[1]NIST, Gaithersburg, MD*

MP 311 **LC/GC Technical Replicates Data Multiplexing Leverages FTMS Applications**; Konstantin O. Nagornov[1]; Anton N. Kozhinov[1]; Florian Albrieux[2]; Carole Reymond[2]; Markus Zennegg[3]; Davide Bleiner[3]; Natalia Gasilova[4]; Laure Menin[5]; Yury O. Tsybin[1]; *[1]Spectroswiss, Lausanne, Switzerland; [2]IFP Energies nouvelles, Solaize, France; [3]Swiss Federal Laboratories for Materials & Technology (EMPA), Dübendorf, Switzerland; [4]Ecole Polytechnique Fédérale de Lausanne, Sion, Switzerland; [5]Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*

MP 312 **High Accuracy Self-Calibration Method for High Resolution Mass Spectra**; Boris Kozlov[1]; Vasily Makarov[2]; Jeffery M. Brown[1]; Keith Richardson[1]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]MS Consulting, Bar, Montenegro*

MP 313 **Investigation of Human Embryo Culture Media Using a Quadrupole Time-Of-Flight (Q-TOF) Mass Spectrometer**; Helen Hao[1]; Evelyn H Wang[2]; Jerry Byrne II[2]; Jennifer Davis[2]; Katie Pryor[2]; Christopher Gilles[2]; *[1]Shimadzu Scientific Instruments, Inc., Columbia, MD; [2]Shimadzu Scientific Instruments, Inc., Columbia, Maryland*

MP 314 **A Chroma Change Study of Acid-Blue 9 Dye with PA12 Powder by UPLC-PDA-HRMSn**; Stone Ouyang[1]; Mark Kowalski[1]; Ali Emamjomeh[1]; Jesiska Tandy[1]; [1]*Hewlett-Packard Company, San Diego, CA*

MP 315 **Qualitative Characterization and Quantitative Assessment of Monoclonal Antibodies Using Protein Metrics and nSMOLTM coupled with the Shimadzu LC-MS 9030 Q-ToF**; Vikki Johnson[1]; Stephen Kurzyneic[2]; [1]*Shimadzu Scientific Instruments, Carlsbad, CA;* [2]*Shimadzu Scientific Instruments, Inc., Columbia, Maryland*

MP 316 **Quantitation of 4,4'-Methylenedianiline and Characterization of Unknown Leachables in Simulated Sweat Migrations Using Liquid Chromatography Quadrupole-TOF Mass Spectrometry**; Noelle Elliott[1]; Marshall Henry[1]; Kate Willis[1]; [1]*Intertek, Allentown, PA*

MP 317 **FTMS Isotopic Simulator: a Like-for-Like Comparison of Experimental and Theoretical Mass Spectra**; Natalia Gasilova[1]; Konstantin O. Nagornov[2]; Anton N. Kozhinov[2]; Laure Menin[3]; Yury Tsybin[2]; [1]*EPFL Valais, Sion, Switzerland;* [2]*Spectroswiss Sàrl, Lausanne, Switzerland;* [3]*EPFL, Lausanne, Switzerland*

MP 318 **High Resolution Quadrupole Mass Spectrometry Analysis for Fusion Reactor and Plasma Facing Materials**; Gregory Thier[1]; Luke Kephart[1]; Jian Wei[1]; [1]*Extrel CMS, Pittsburgh, PA*

MP 319 **Evaluation of Orbitrap and Time-of-Flight Mass Analyzers for High-Throughput Metabolomics**; Michelle Reid[1]; Tobias Fuhrer[1]; Nicola Zamboni[1]; [1]*ETH Zurich, Zurich, Switzerland*

MP 320 **Extractables & Leachables Analysis Using the Hi-Resolution Accurate Mass GC/QTOF**; Thomas S Talwar[1]; Matthew Curtis[2]; [1]*Agilent Technologies, Inc., Wilmington, DE;* [2]*Agilent Technologies, Inc., Santa Clara, CA*

MP 321 **Molecular Structure Study of Polyether Polyols by UPLC-QTOF MS**; Junyan Liu; *Sinopec Shanghai Research Institute of Petrochemical Technology, Shanghai, China*

MP 322 **Simultaneous Profile and Determination of Statin Composition in Various Media and Biological Matrices by Accurate Mass and High Resolution LC-QTOF-MS**; Wei Chen[1]; Patrick Lin[1]; Bih Hsu[1]; Zicheng Yang[2]; Xuejun Peng[2]; Guillaume Tremintin[2]; [1]*Pharmout Laboratory, Fremont, CA;* [2]*Bruker Daltonics, San Jose, CA*

MP 323 **Critical Comparison of Fourier Transform Mass Spectrometry Platforms for Metabolite Elemental Formula Elucidation Purposes**; Danning Huang[1]; Marcos Bouza Areces[1]; David Gaul[1]; Arthur S. Edison[2]; Facundo M. Fernandez[1]; [1]*Georgia Institute of Technology, Atlanta, GA;* [2]*University of Georgia, Athens, GA*

MP 324 **Sensitive Perfluoroalkyl Substance (PFAS) Screening Using High Resolution Accurate Mass Spectral Library**; Gerard Byrne[1]; Brahm Prakash[1]; Evelyn Wang[1]; Christopher Gilles[1]; [1]*Shimadzu Scientific Instruments, Inc., Columbia, MD*

MP 325 **Untargeted Metabolomics and 13C-Labeling in Tissue Culture for Identifying Unknown Human Biotransformation Products of Xenobiotics**; Mira Flasch[1]; Christoph Bueschl[2]; Lydia Woelfingseder[1]; Rainer Schuhmacher[2]; Doris Marko[1]; Benedikt Warth[1,3,4]; [1]*University of Vienna, Faculty of Chemistry, Department of Food Chemistry and Toxicology, Vienna, Austria;* [2]*University of Natural Resources and Life Sciences, Department of Agrobiotechnology, Center for Analytical Chemistry, IFA-Tulln, Vienna, Austria;* [3]*Research Network Chemistry Meets Microbiology, University of Vienna, Vienna, Austria;* [4]*Vienna Metabolomics Center (VIME), Vienna, Austria*

MP 326 **Facile Generation of Absorption-Mode Mass Spectra on FT-ICR MS Instruments**; Anton N. Kozhinov[1]; Konstantin O. Nagornov[1]; Yury O. Tsybin[1]; [1]*Spectroswiss, Lausanne, Switzerland*

MP 327 **Using TOF-MS to Improve Quality in High Throughput Laboratories**; Lucas Marshall, MS[1]; Jason Hull, MS[1]; Rebecca Heltsley, PhD[1]; [1]*Aegis Sciences Corporation, Nashville, TN*

MP 328 **Developments in Orbitrap Mass Spectrometry on a Modified Tribrid Mass Spectrometer**; Jesse D. Canterbury[1]; Graeme McAlister[1]; Michael W. Senko[1]; Romain Huguet[1]; Aaron Robitaille[1]; Arne Kreutzmann[2]; Daniel Mourad[2]; Konstantin Aizikov[2]; Dmitry Grinfeld[2]; Alexander Makarov[2]; [1]*Thermo Fisher Scientific, San Jose, CA;* [2]*Thermo Fisher Scientific, Bremen, Germany*

MP 329 **Targeted Screening of Coumarins and Furanocoumarins in Essential Oils Utilizing Accurate Mass on a High-Resolution Quadrupole Time-of-Flight Mass Spectrometer**; Jennifer C Davis[1]; Evelyn H Wang[1]; Katie Pryor[1]; Gerard Byrne[1]; Helen Hao[1]; Christopher Gilles[1]; [1]*Shimadzu Scientific Instruments, Inc., Columbia, Maryland*

MP 330 **Suspect Screening for Antimicrobials and Other Micropollutants in Wastewater and Surface Waters from Asia using High Resolution Mass Spectrometry**; Diana Aga[1]; Luisa Angeles[1]; [1]*University at Buffalo, Buffalo, NY*

MP 331 **Advanced Proteomics Quality Control Samples for Assessing Reversed-Phase Liquid Chromatography Tandem Mass Spectrometry Performance Metrics**; Jaclyn Gowen Kalmar[1]; Michael S. Bereman[1]; David C Muddiman[1]; [1]*North Carolina State University, Raleigh, NC*

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MP 332 **Co-registration and Analysis of MALDI and Confocal Fluorescence Images of Stem Cell Colonies via Multivariate Regression**; Arina A Nikitina[1]; Danning Huang[2]; Sarah Seals[3]; Li Li[2]; Melissa Kemp[3]; Facundo M Fernandez[2]; [1]*School of Biological Sciences, Georgia Institute of Technology, Atlanta, GA;* [2]*School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA;* [3]*The Wallace H. Coulter Department of Biomedical Engineering, Georgia Institute of Technology and Emory University, Atlanta, GA*

MP 333 **Dissimilarity Metrics Mapping Algorithm for Assist Region Detection in Mass Spectrometry Imaging**; Evgeny Zhvansky[1]; Anatoly Sorokin[1,2]; Daniil Ivanov[1]; Vasiliy Eliferov[1]; Anna Bugrova[3]; Stanislav Pekov[1,4]; Igor Popov[1,4]; Eugene (evgeny) Nikolaev[5]; [1]*Moscow Institute of Physics and Technology (State University), Dolgoprudny, Russia;* [2]*Institute of Cell Biophysics RAS, Pushchino, Russia;* [3]*Institute of Biochemical Physics RAS, Moscow, Russia;* [4]*Institute for Energy Problems of Chemical Physics RAS, Moscow, Russia;* [5]*Skolkovo institute of science and technology, Moscow Region, Russian Federation*

MP 334 **Automatic Identification of Suborgan Regions in MS Imaging**; Laura Castellanos-García[1]; Richard W. Vachet[1]; [1]*University of Massachusetts, Amherst, MA*

MP 335 **Development and Benchmarking of Automated, Computational Registration of Microscopy and MALDI Imaging Mass Spectrometry Datasets**; Heath Patterson[1]; Michael D. Tuck[2]; Martin Dufresne[2,3]; Richard M. Caprioli[2,3,4]; [1]*Vanderbilt University, Nashville, TN;* [2]*Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN;* [3]*Department of Biochemistry, Vanderbilt University, Nashville, TN;* [4]*Department of Chemistry, Vanderbilt University, Nashville, TN*

MP 336 **Automated MS Imaging Data Processing Pipeline for Routine and Creative Data Explorations: from Data Acquisition to Archiving**; Teresa Murta[1]; Spencer A. Thomas[1]; Alex Dexter[1]; Ala Al-Afeef[1]; Adam J. Taylor[1]; Bin Yan[1]; Chelsea J. Nikula[1]; Efstathios Elia[1]; Kenneth N. Robinson[1]; Rory T. Steven[1]; Tingting Fu[1]; Weiwei Zhou[1];

Xavier Loizeau[1]; Josephine Bunch[1,2]; [1]*National Physical Laboratory, London, United Kingdom;* [2]*Imperial College, London, United Kingdom*

MP 337 **Fully Automated Mass Alignment and Recalibration of MALDI TOF Imaging Data from N-Linked Glycans**; Tobias Boskamp[1,2]; Alyson Black[3]; Anand Mehta[3]; Richard Drake[3]; Yujin Hoshida[4]; Dennis Trede[1]; Peter Maass[1,2]; [1]*SCiLS, Bremen, Germany;* [2]*University of Bremen, Bremen, Germany;* [3]*Medical University of South Carolina, Charleston, SC;* [4]*University of Texas Southwestern Medical Center, Dallas, TX*

MP 338 **An Ion Mobility Quadrupole Time of Flight Mass Spectrometry Imaging Workflow**; Daniela Mesa Sanchez[1]; Stephen Creger[1]; Ruwan T Kurulugama[2]; John C. Fjeldsted[2]; Julia Laskin[1]; [1]*Purdue University, West Lafayette, IN;* [2]*Agilent Technologies, Inc., Santa Clara, CA*

MP 339 **Co-Registered Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry and Time-of-Flight Secondary Ion Mass Spectrometry Data for Visualizing Sub-cellular Brain Signaling Pathways**; Steven T King[1]; Matthias Lorenz[1]; Nikolay Borodinov[1]; Junghoon Chae[1]; Chad A Steed[1]; Anton V. Ievlev[1]; Olga S Ovchinnikova[1]; [1]*Oak Ridge National Laboratory, Oak Ridge, TN*

MP 340 **Optimized Data Analysis Pipeline for MALDI Imaging Based Tumor Typing from FFPE Tissue Samples Evaluated on Six Benchmark Classification Tasks**; Delf Lachmund[1]; Jonathan von Schroeder[1]; Tobias Boskamp[1,2]; Lena Hauberg-Lotte[1]; Jan H. Kobarg[2]; Sören-Oliver Deininger[3]; Katharina Kriegsmann[4]; Mark Kriegsmann[4]; Rita Casadonte[5]; Jörg Kriegsmann[5]; Peter Maass[1,2]; [1]*University of Bremen, Bremen, Germany;* [2]*SCiLS, Bremen, Germany;* [3]*Bruker Daltonik GmbH, Bremen, Germany;* [4]*University of Heidelberg, Heidelberg, Germany;* [5]*Proteopath, Trier, Germany*

MP 341 **Co-Registered MALDI and ToF-SIMS Data for Visualizing Sub-cellular Signaling Pathways in the Brain**; Matthias Lorenz[1]; Stephen T. King[1]; Chad A. Steed[1]; Junghoon Chae[1]; Anton V. Ievlev[1]; Olga S. Ovchinnikova[1]; [1]*Oak Ridge National Laboratory, Oak Ridge, TN*

MP 342 **Unsupervised Segmentation of Mass Spectrometric Ion Images Characterizes Morphology of Tissues**; Dan Guo[1]; Kylie Bemis[1]; Catherine Rawlins[1]; Jeffery Agar[1]; Olga Vitek[1]; [1]*Northeastern University, Boston, MA*

IMAGING MS: INSTRUMENTATION
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MP 343 **High Efficiency Miniature Imaging Mass Spectrometer**; Xiangyu Guo[1]; Wenbo Cao[1]; Xiaoxiao Ma[1]; Xinwei Liu[1]; Zheng Ouyang[1,2]; [1]*State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China;* [2]*Weldon School of Biomedical Engineering and Department of Chemistry, Purdue University, West Lafayette, IN*

MP 344 **21 T MALDI FT-ICR Mass Spectrometry for High Performance Molecular Imaging**; Donald F. Smith[1]; Andrew P. Bowman[2]; Shane R. Ellis[2]; Greg T. Blakney[1]; Ron M. A. Heeren[2]; Christopher L. Hendrickson[1,3]; [1]*National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL;* [2]*Maastricht Multimodal Molecular Imaging (M4I) Institute, Division of Imaging Mass Spectrometry, Maastricht, Netherlands;* [3]*Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL*

MP 345 **Observation on Regeneration Behavior of Zebrafish Caudal Fin Using High-Spatial Resolution Mass Spectrometric Imaging**; Jae Young Kim[1]; Sun Young Lee[1]; Ji-Won Park[2]; Dong-Kwon Lim[3]; Dae Won Moon[1]; [1]*Daegu Gyeongbuk Institute of Science and Technology, Daegu, South Korea;* [2]*Chungnam National University, Daejeon, South Korea;* [3]*Korea University, Seoul, South Korea*

MP 346 **Optimized Rapid Matrix Sublimation Device for MALDI Mass Spectrometry Imaging**; Vasily Eliferov[1]; Daniil Ivanov[1]; Andrey Shivalin[1]; Igor Popov[1,2]; Eugene (Evgeny) Nikolaev[3]; [1]*Moscow Institute of Physics and Technology (State University), Dolgoprudny, Russia;* [2]*Institute of Biochemical Physics RAS, Moscow, Russia;* [3]*Skolkovo institute of science and technology, Moscow Region, Russian Federation*

MP 347 **Upgrade of an LTQ-Orbitrap XL MALDI Source for High Spatial Resolution in Image Experiments**; Raul Montero[1]; Lucía Martín-Saiz[1]; Jone Garate[1]; Beatriz Abad-García[1]; Jose A Fernandez[2]; [1]*University of the Basque Country, Leioa, Spain;* [2]*Universidad del Pais Vasco, Leioa, Spain*

MP 348 **Characteristics of MALDI-Imaging on a New Dual Ion Source QTOF with TIMS Separation**; Arne Fuetterer[1]; Juergen Suetering[1]; Janina Oetjen[1]; Niels Goedecke[1]; Stephanie Kaspar-Schoenefeld[1]; Scarlet Koch[1]; Shannonn Cornett[2]; Alice Ly[1]; Jens Fuchser[1]; Lucy Woods[1]; Oliver Raether[1]; Jens Hoehndorf[1]; [1]*Bruker Daltonik GmbH, Bremen, Germany;* [2]*Bruker Daltonics Inc., Billerica, MA*

MP 349 **Atmospheric Pressure Mass Spectrometry Imaging with Post-Ionisation**; Rory Thomas Steven[1]; Kenneth N. Robinson[1]; Alex Dexter[1]; Michael Shaw[1]; Teresa Murta[1]; Bin Yan[1]; Weiwei Zhou[1]; Ian S Gilmore[1]; Zoltan Takats[2]; Josephine Bunch[1,2]; [1]*National Physical Laboratory, London, United Kingdom;* [2]*Imperial College London, London, United Kingdom*

MP 350 **High-Resolution Ion Microscope Imaging over Broad Mass Ranges Using a Reflectron**; Michael Burt[1]; Robert Burleigh[1]; Ang Guo[1]; Fei Gao[1]; Natasha Smith[1]; Mark Brouard[1]; [1]*University of Oxford, Oxford, United Kingdom*

MP 351 **Gas-Phase Charge Inversion Ion/Ion Reactions on an FT-ICR Mass Spectrometer for Fatty Acids Identification in Imaging Mass Spectrometry**; Julia R Bonney[1]; Xizheng Diao[1]; Steve L. Van Orden[2]; Boone M. Prentice[1]; [1]*University of Florida Department of Chemistry, Gainesville, FL;* [2]*Bruker Daltonics Inc., Billerica, MA*

MP 352 **Co-Registered, Cellular-Resolution Mass Spectrometry and Fluorescence Imaging for the Multi-Omic Targeting of Rare Cell Types**; Eric C. Spivey[1,2]; Josiah C. McMillen[1,3]; David M. Anderson[1]; Daniel J. Ryan[1,3]; Jeffrey M. Spraggins[1,3,4]; John P. Wikswo[2,5,6]; Richard M. Caprioli[1,3,4]; Jeremy L. Norris[1,4]; [1]*Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN;* [2]*Vanderbilt University Department of Biomedical Engineering, Nashville, TN;* [3]*Vanderbilt University Department of Chemistry, Nashville, TN;* [4]*Vanderbilt University Department of Biochemistry, Nashville, TN;* [5]*Vanderbilt Institute for Integrative Biosystems Research and Education, Nashville, TN;* [6]*Vanderbilt University Department of Physics, Nashville, TN*

MP 353 **MALDI Spatial Resolution Improvement Using MALDI-2 Post-Ionization**; Josiah C. McMillen[1,2]; Eric C. Spivey[2,3]; Daniel J. Ryan[1,2]; Jeffrey M. Spraggins[1,2,4]; Richard M. Caprioli[1,2,4,5,6]; [1]*Department of Chemistry, Vanderbilt University, Nashville, TN;* [2]*Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN;* [3]*Department of Biomedical Engineering, Vanderbilt University, Nashville, TN;* [4]*Department of Biochemistry, Vanderbilt University, Nashville, TN;* [5]*Department of Pharmacology, Vanderbilt University, Nashville, TN;* [6]*Department of Medicine, Vanderbilt University, Nashville, TN*

MP 354 **Sub-Cellular Chemical and Functionals Imaging AFM-MS and Analysis of Biological Tissues**; Ryan Wagner[1]; Matthias Lorenz[2]; Olga S Ovchinnikova[3]; Roger Proksch[1]; [1]*Oxford Instruments, Santa Barbara, CA;* [2]*University of Tennessee / Oak Ridge National Laboratory, Oak Ridge, TN;* [3]*Oak Ridge National Laboratory, Oak Ridge, TN*

MP 355 **Characterization of a Prototype MALDI timsTOF Pro for High-Performance Imaging Mass Spectrometry**; Katerina V Djambazova[1,2]; Lukasz Migas[3]; Nathan Heath Patterson[2,

[4]; Raf Van de Plas[3]; Richard M. Caprioli[1,2,4,5,6]; Jeffrey M. Spraggins[1,2,4]; [1]*Department of Chemistry, Vanderbilt University, Nashville, TN;* [2]*Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN;* [3]*Delft Center for Systems and Control, Delft University of Technology, Delft, Netherlands;* [4]*Department of Biochemistry, Vanderbilt University, Nashville, TN;* [5]*Department of Medicine, Vanderbilt University, Nashville, TN;* [6]*Department of Pharmacology, Vanderbilt University, Nashville, TN*

MP 356 **Development of High Spatial Resolution and High Speed Projection-type Imaging Mass Spectrometor**; Jun Aoki[1]; Michisato Toyoda[1]; [1]*Osaka University, Toyonaka, Japan*

MP 357 **Coupling IR-MALDESI and Ion Mobility-Mass Spectrometry for Rapid Isomer Distinction in Imaging Experiments**; Måns Ekelöf[1]; James N. Dodds[1]; Jeffrey G. Manni[2]; Kenneth P. Garrard[1]; Sitora Khodjaniyazova[1]; Erin S Baker[1]; David C. Muddiman[1]; [1]*North Carolina State University, Raleigh, NC;* [2]*JGM Associates, Burlington, MA*

MP 358 **Understanding the Role of Electrospray Solvent Composition on the Ionization of Diverse Chemical Classes by IR-MALDESI MSI**; Måns Ekelöf[1]; David C Muddiman[1,2]; Michael C. Bagley[1]; Liana Gouveia[1]; [1]*North Carolina State University, Raleigh, NC;* [2]*Molecular Education, Technology, and Research Innovation Center (METRIC), North Carolina State University, Raleigh, NC*

MP 359 **RastirX: A Versatile Platform for Imaging Arbitrary Spatial Patterns**; Kenneth P. Garrard[1,2]; Måns Ekelöf[1]; Sitora Khodjaniyazova[1]; Michael C. Bagley[1]; David C. Muddiman[1,3]; Elias P. Rosen[4]; William M. Gilliland, Jr.[4]; Angela D. M. Kashuba[4]; [1]*FTMS Laboratory for Human Health Research, Department of Chemistry, North Carolina State University, Raleigh, NC;* [2]*Precision Engineering Consortium, North Carolina State University, Raleigh, NC;* [3]*Molecular Education, Technology, and Research Innovation Center (METRIC), North Carolina State University, Raleigh, NC;* [4]*Division of Pharmacotherapy and Experimental Therapeutics, University of North Carolina at Chapel Hill, Chapel Hill, NC*

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MP 360 **A Quantitative Evaluation of Ion Chromatogram Extraction Algorithms**; Annika Tostengard[1]; Robert Smith[2]; [1]*The University of Montana, Missoula, MT;* [2]*University of Montana Missoula, Missoula, MT*

MP 361 **LipidAnalyst: A Deep Neural Network Approach for Standardized and Comprehensive Lipidomic Analysis**; Naren Gajenthra Kumar[1]; Aliakbar Panahi[2]; Joseph J Nalluri[3]; Dayanjan S Wijesinghe[2]; [1]*Department of Microbiology and Immunology, Virginia Commonwealth University, Richmond, VA;* [2]*Department of Pharmacotherapy and Outcomes Sciences, Virginia Commonwealth University, Richmond, VA;* [3]*Department of Radiation Oncology, Virginia Commonwealth University, Richmond, VA*

MP 362 **AP3: An Advanced Proteotypic Peptide Predictor for Targeted Proteomics by Integrating Peptide Digestion Probability**; Zhiqiang Gao[1]; Cheng Chang[2,3]; Yan Fu[1]; [1]*NCMIS, RCSDS, Academy of Mathematics and Systems Science, Chinese Academy of Sciences, Beijing, China;* [2]*Beijing Institute of Lifeomics, Beijing, China;* [3]*Beijing Proteome Research Center, Beijing, China*

MP 363 **Focus on the Spectra that Matter by Clustering of Quantification Data in Shotgun Proteomics**; Matthew The[1]; Lukas Kall[1]; [1]*Royal Institute of Technology, Stockholm, Sweden*

MP 364 **Predicting Optimal Values of Parameters for Peak Deconvolution Using a Convolutional Neural Network**; Yuichiro Fujita[1]; Akira Noda[1]; Yohei Yamada[1]; Katsuyuki Taneda[1]; Junko Iida[1,2]; Shigeki Kajihara[1]; [1]*Shimadzu Corporation, Kyoto, Japan;* [2]*Osaka University Shimadzu Analytical Innovation Research Laboratory, Suita, Japan*

MP 365 **Simulated Impacts of Mass Resolving Power on the Resulting Mass Error Distribution in Mass Spectrometry Analysis**; Melaine Q Couch[1]; Martha L. Chacón-Patiño[1]; Christopher L. Hendrickson[1,2]; Yuri E. Corilo[1]; [1]*National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL;* [2]*Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL*

MP 366 **Predicting Ion Mobility Collision Cross Sections by Combining Conventional and Data Driven Modelling**; Robbin Bouwmeester[1,2]; Lennart Martens[1,2]; Sven Degroeve[1,2]; Keith Richardson[3]; Johannes PC Vissers[3]; [1]*VIB-UGent Center for Medical Biotechnology, Ghent, Belgium;* [2]*Department of Biochemistry, Ghent University, Ghent, Belgium;* [3]*Waters Corporation, Wilmslow, United Kingdom*

MP 367 **A New Spectral Baseline Subtraction Algorithm for Reducing Artefacts in Protein Deconvolution**; Lyle Burton[1]; Xu Guo[1]; Gordana Ivosev[1]; Ron Bonner[2]; [1]*SCIEX, Concord, ON;* [2]*Ron Bonner Consulting, Newmarket, ON*

MP 368 **Toffee: A Highly Compressed, Efficient, File Format for DIA-MS**; David Clarke[1]; Akila Seneviratne[1]; Brett Tully[1]; [1]*ProCan, Children's Medical Research Institute, The University of Sydney, Westmead, Australia*

MP 369 **Increased Peptide Detection Accuracy in DIA-MS via Chemical and Random Additive Noise Elimination (Crane)**; Akila J Seneviratne[1]; Brett Tully[1]; [1]*ProCan, Children's Medical Research Institute, The University of Sydney, Westmead, Australia*

MP 370 **Exploring DIA Proteomics Spectra with Tensor-based Deconvolution**; Filip Buric[1]; Aleksej Zelezniak[1,2]; [1]*Chalmers University of Technology, Gothenburg, Sweden;* [2]*Science for Life Laboratory, KTH - Royal Institute of Technology, Stockholm, Sweden*

MP 371 **Repeat-Preserving Decoy Database for False Discovery Rate Estimation in Peptide Identification**; Johra Muhammad Moosa[1]; Shenheng Guan[1,2]; Michael F. Moran[2,3]; Bin Ma[1]; [1]*David R. Cheriton School of Computer Science, University of Waterloo, Waterloo, ON;* [2]*Program in Cell Biology and SPARC BioCentre, Hospital for Sick Children, Toronto, ON;* [3]*Department of Molecular Genetics, University of Toronto, Toronto, ON*

MP 372 **MS-PROTINI: A Protein-Protein Interaction-Assisted Algorithm for the Confidence Assessment of Peptide and Protein Identifications in Mass Spectrometry-Based Proteomics**; Francesca A. Barry[1]; Zhibin Ning[1]; Daniel Figeys[1]; Mathieu Lavallée-adam[1]; [1]*University of Ottawa, Ottawa, ON*

MP 373 **Peptide Migration Time Prediction in Capillary Zone Electrophoresis Mass Spectrometry Using a Convolutional Neural Network Model**; Wenrong Chen[1]; Liangliang Sun[2]; Xiaowen Liu[1,3]; [1]*Department of BioHealth Informatics, Indiana University-Purdue University Indianapolis, Indianapolis, Indiana;* [2]*Department of Chemistry, Michigan State University, East Lansing, 48824;* [3]*Center for Computational Biology and Bioinformatics, Indiana University School of Medicine, Indianapolis, IN*

MP 374 **A Novel Algorithm for Automating Fragment Ion Structure Assignment Using High Mass Accuracy MS/MS data**; Neil Loftus[1]; Kirsten Hobby[1]; Alan Barnes[1]; [1]*Shimadzu Corporation, Manchester, United Kingdom*

MP 375 **Factor Analysis Identifies Biologically Meaningful Proteoform Families of Human ApoA-I**; Richard LeDuc[1]; Henrique Seckler[2]; John T Wilkins[2]; Ryan T Fellers[2]; Joseph B Greer[2]; Paul M Thomas[2]; Neil L Kelleher[2]; [1]*Northwestern*

University, Bloomington, IN; [2]Proteomics Center of Excellence, Northwestern University, Chicago, IL

MP 376 **GPU-Based Signal Processing Optimization for 1&2D FT-ICR Mass Spectrometer Data**; Marc Haegelin[1]; Fabrice Bray[1]; Anne Jeannin-Girardon[2]; Pierre Collet[2]; Christian Rolando[1]; *[1]Université de Lille, Villeneuve d'Ascq, France; [2]Université de Strasbourg, Strasbourg, France*

MP 377 **Masstodon: A Tool for in Depth Analysis of your Mass Spectrum**; Maleusz Krzysztof Lacki[1]; Frederik Lermyte[2, 3, 4]; Błażej Miasojedow[5]; Michał Piotr Startek[5]; Stefan Tenzer[1]; Frank Sobott[2, 6, 7]; Dirk Valkenborg[3, 8, 9]; Anna Gambin[5]; *[1]University Medical Center Mainz, Mainz, Germany; [2]Biomolecular and Analytical Mass Spectrometry group, University of Antwerp, Belgium; [3]Centre for Proteomics (University of Antwerp/VITO (Belgium)), Antwerpen, Belgium; [4]School of Engineering, University of Warwick, Coventry, United Kingdom; [5]University of Warsaw, Warsaw, Poland; [6]Astbury Centre for Structural Molecular Biology, University of Leeds, United Kingdom; [7]School of Molecular and Cellular Biology, University of Leeds, United Kingdom; [8]Flemish Institute for Technological Research (VITO), Mol, Belgium; [9]Interuniversity Institute for Biostatistics ans Statistical Bioinformatics, Hasselt, Belgium*

MP 378 **Using Isotopic Cluster, Neutral Loss and Adduct Analyses to Improve Component Detection in LC HRAM MS Experiment**; Juraj Lutisan[1]; Michal Grambličkа[1]; Žofia Lutišanová[1]; Robert Mistrik[1]; Xiaojie C. Ding[2]; Vladimír Pätoprstý[3]; *[1]HighChem, Bratislava, Slovakia; [2]Thermo Fisher Scientific, San Jose, CA; [3]Slovak Academy of Sciences, Bratislava, Slovakia*

MP 379 **Automated Predicting Fragmentation Scheme for Molecules during Collision-Induced Dissociation**; Grzegorz Skoraczynski[1]; Michal Ciach[1, 2]; Michal Startek[1]; Anna Gambin[1]; *[1]Faculty of Mathematics, Informatics and Mechanics, University of Warsaw, Warsaw, Poland; [2]Centrum voor Statistiek, Hasselt University, Diepenbeek, Belgium*

MP 380 **An Efficient Method for Cosine Similarity Threshold Search Using a Peak Indexing Strategy**; Jonghun Park[1]; Yuliang Li[1]; Jianguo Wang[1]; Benjamin Pullman[1]; Yannis Papakonstantinou[1]; Nuno Bandeira[1]; *[1]UC San Diego, La Jolla, CA*

MP 381 **Bioinformatics Optimization Approaches for the Label-Free Quantitation of Ubiquitinated Peptides in Bottom-Up MS-Based Proteomics**; Arzu Tugce Guler[1]; Karen A. Sap[1]; Aleksandra Bury[1]; Karel Bezstarosti[2]; Jeroen A.A. Demmers[2]; Eric A. Reits[1]; *[1]Amsterdam UMC, Amsterdam, Netherlands; [2]Erasmus MC, Rotterdam, Netherlands*

MP 382 **Using Generalized Chemical Artificial Intelligence to Calculate Molecular Properties, Including GC Retention Indices**; Lewis Geer[1]; Stephen E. Stein[1]; William E. Wallace[1]; *[1]NIST, Gaithersburg, MD*

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MP 383 **Prosit: Investigating Vast and Complex Peptide Spaces by Boosting Identification Confidence through Highly-Accurate Fragment Intensity Predictions**; Siegfried Gessulat[1, 2]; Tobias Schmidt[1]; Daniel P Zolg[1]; Julia Rechenberger[1]; Patroklos Samaras[1]; Steven Verbruggen[3, 4]; Bernard Delanghe[5]; Andreas Huhmer[6]; Karsten Schnatbaum[7]; Ulf Reimer[7]; Hans-Christian Ehrlich[2]; Stephan Aiche[2]; Gerben Menschaert[3, 4]; Bernhard Kuster[1, 8, 9]; Mathias Wilhelm[1]; *[1]Technical University of Munich, Freising, Germany; [2]SAP SE, Potsdam, Germany; [3]Ghent University, Ghent, Belgium; [4]BioBix Lab, Ghent, Belgium; [5]Thermo Fisher Scientific, Bremen, Germany; [6]Thermo Fisher Scientific, San Jose, CA; [7]JPT Peptide Technologies GmbH, Berlin, Germany; [8]Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany; [9]Center for Integrated Protein Science Munich, Freising, Germany*

MP 384 **Improved Algorithms for Identifying Phosphopeptides in Peptide Tandem Mass Spectral Libraries**; Sergey Sheetlin[1]; Dmitrii V. Tchekhovskoi[1]; Zheng Zhang[1]; Stephen E. Stein[1]; *[1]NIST, Gaithersburg, MD*

MP 385 **The Mouse Quantitative Proteomics Knowledge Base: CPTAC-Validated Quantitative Targeted Proteomics Assays for Discovery in Mouse Models**; Yassene Mohammed[1, 2]; Pallab Bhowmick[1]; Sarah A. Michaud[1]; Helena Pětrošová[1]; Christoph H. Borchers[1, 3, 4, 5]; *[1]University of Victoria-Genome BC Proteomics Centre, Victoria, BC; [2]Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; [3]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; [4]Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; [5]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC*

MP 386 **Targeted Proteomics Assays for FDA-Approved Protein Biomarkers**; Yassene Mohammed[1, 2]; Simon Roome[1]; Pallab Bhowmick[1]; Christoph H. Borchers[1, 3, 4, 5]; *[1]University of Victoria-Genome BC Proteomics Centre, Victoria, BC; [2]Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; [3]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; [4]Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; [5]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC*

MP 387 **Peak Finding and Quantification Improvements in Skyline**; Nicholas Shulman[1]; Brian C Searle[2, 3]; Micheal J MacCoss[1]; Brendan X MacLean[1]; *[1]University of Washington, Seattle, WA; [2]Systems Biology, Seattle, WA; [3]Proteome Software, Portland, OR*

MP 388 **Bonfire Search Engine for Precursor-Independent Identification of Peptides with Exact or Open Modification to Uncover the "Dark Proteome"**; Wen Yu[1]; Raghothama Chaerkady[1]; Xiaotao Qu[1]; Sonja Hess[1]; David A Fenstermacher[1]; *[1]MedImmune, Gaithersburg, MD*

MP 389 **ImmuNOVO: A Software Tool for Constrained *de novo* Sequencing of Neo-Epitope Peptides from Immunopeptideomics**; Sujun Li[1]; Haixu Tang[2]; *[1]Indiana University, Bloomington, IN; [2]Indiana University Bloomington, Bloomington, IN*

MP 390 **Extremely Efficient Open Modification Spectral Library Searching Using Spectrum Hashing and GPUs Allows Large-Scale PTM Profiling**; Wout Bittremieux[1, 2]; Kris Laukens[2]; William Stafford Noble[1]; *[1]University of Washington, Seattle, WA; [2]University Of Antwerp, Antwerp, Belgium*

MP 391 **Improving Peptide Identification by Library Search from Chimeric Spectra**; Wenju Zhang[1]; Zhewei Liang[1]; Xin Chen[1]; Lei Xin[1]; Baozhen Shan[1]; *[1]Bioinformatics Solutions Inc., Waterloo, ON*

MP 392 **A New Feature-Based Workflow Unifies DDA and DIA Data Analysis**; Wen Zhang[1]; Weiping Sun[1]; Ziaur Rahman[1]; Yi Liu[1]; Lei Xin[1]; *[1]Bioinformatics Solutions Inc., Waterloo, ON*

MP 393 **Identification of Inconsistent Peptide Recovery and Aberrant Peptide Termini as Sources of Sample Variability in Patient-derived Tumor Samples**; Meghan Burke[1]; Zheng Zhang[1]; Yuri A. Mirokhin[1]; Dmitrii V. Tchekhovskoi[1]; Stephen E. Stein[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

MP 394 **Robust Cross-Linked Peptide Detection Using Pretrained Neural Networks**; William E Fondrie[1]; William Stafford Noble[1]; [1]*The University of Washington, Seattle, WA*

MP 395 **Validation of Peptide Identification Using Housekeeping Genes as Positives in Supervised Learning**; Honglan Li[1]; Seungjin Na[1]; Kyu-Baek Hwang[2]; Eunok Paek[1]; [1]*Hanyang University, Seoul, South Korea;* [2]*Soongsil University, Seoul, South Korea*

MP 396 **Ion Mobility Enhanced Matching between LC-MS Runs and Collisional Cross Section Prediction Improve Identification and Quantification in MaxQuant**; Nikita Prianichnikov[1]; Favio Salinas Soto[1]; Heiner Koch[2]; Scarlet Koch[2]; Markus Lubeck[2]; Sven Brehmer[2]; Juergen Cox[1]; [1]*Max Planck Institute of Biochemistry, Martinsried, Germany;* [2]*Bruker Daltonik GmbH, Bremen, Germany*

MP 397 **phosMS-GF+: Database Dependent Search Engine for Improved Phosphopeptide Identifications**; Daniela M Schlatzer[1]; Sean Maxwell[2]; Mark R. Chance[1]; [1]*Center for Proteomics and Bioinformatics, CWRU, Cleveland, Ohio;* [2]*Case Western Reserve University, Cleveland, OH*

MP 398 **Automating Distributed Analysis of Large MS/MS Datasets**; Julie S Wertz[1]; Jeremy Carver[1]; Nuno Bandeira[1]; [1]*University of California San Diego, La Jolla, CA*

MP 399 **Indexed Retention Time (iRT) Prediction of Peptides by Deep Learning**; Shenheng Guan[1,2]; Jia Rong Wu[1]; Michael F. Moran[2,3]; Bin Ma[1]; [1]*University of Waterloo, Waterloo, ON;* [2]*SPARC BioCentre, Hospital for Sick Children, Toronto, Ontario;* [3]*University of Toronto, Toronto, Ontario*

MP 400 **Improved Label-Free Quantification with MaxQuant through more Robust Feature Alignment**; Mai Sun[1]; Xuemei Zeng[1]; Nathan A. Yates[1,2]; [1]*Biomedical Mass Spectrometry Center, University of Pittsburgh Schools of the Health Sciences, Pittsburgh, PA;* [2]*Department of Cell Biology, University of Pittsburgh School of Medicine, Pittsburgh, PA*

MP 401 **Bolt: A New Age Peptide Search Engine for Comprehensive MS/MS Sequencing through Vast Protein Databases in Minutes**; Amol Prakash[1]; Swetaketu Majumder[1]; Shadab Ahmad[1]; Conor Jenkins[2]; Benjamin Orsburn[3]; [1]*Optys Tech Corporation, Shrewsbury, MA;* [2]*Hood College Bioinformatics Program, Frederick, MD;* [3]*National Cancer Institute @ Frederick, Frederick, MD*

MP 402 **Comparison of Open-Search Tools**; Fengchao Yu[1]; Guo-Ci Teo[1]; Andy T. Kong[1]; Felipe V. Leprevost[1]; Hui-Yin Chang[1]; Alexey I. Nesvizhskii[1]; [1]*University of Michigan, Ann Arbor, MI*

MP 403 **METATRYP 2.0: Improvements in METATRYP Software for Metaproteomic Least Common Ancestor Analyses within the Ocean Protein Portal**; David Gaylord[1]; Jaclyn Saunders[1]; Noelle Held[1]; Nick Symmonds[1]; Adam Shepherd[1]; Michael Chagnon[2]; Danie Kinkade[1]; Tom Delmont[3]; A. Murat Eren[3]; Chris Dupont[4]; Mak Saito[1]; [1]*Woods Hole Oceanographic Institution, Wood Hole, MA;* [2]*RPS Ocean Science, South Kingston, RI;* [3]*University of Chicago, Chicago, IL;* [4]*J. Craig Venter Institute, La Jolla, CA*

MP 404 **Exploring Phosphopeptide Variability across Search Engines and Parameters**; Bhoomi Bhatt[1]; Alexander Saltzman[1]; Mei Leng[1]; Antrix Jain[1]; Anna Malovannaya[1]; [1]*Baylor College of Medicine, Houston, Texas*

MP 405 **Shifted Ions Searching and Other Improvements in the MSFragger Database Search Engine**; Guo Ci Teo[1]; Andy T. Kong[1]; Hui-Yin Chang[1]; Felipe Da Veiga Leprevost[1]; Dmitry Avtonomov[1]; Alexey I. Nesvizhskii[1]; [1]*University of Michigan, Ann Arbor, MI*

MP 406 **Prediction of z+1 Hydrogen Rearrangement in ETD Spectra**; Jia R Wu[1]; Bin ma[1]; Shenheng Guan[1]; [1]*University of Waterloo, Waterloo, ON*

MP 407 **Open Modification Analysis of Keratin Proteins in Hair and Skin Samples**; Brett S Phinney[1]; Michelle R Salemi[1]; Glendon J Parker[2]; Zachary C Goecker[2]; Robert H Rice[2]; [1]*Proteomics Core Facility, UC Davis Genome Center, University of California, Davis, Davis, CA;* [2]*Department of Environmental Toxicology, University of California, Davis, CA, Davis, CA*

MP 408 **The Sushi Proteome Project towards Unveiling Dietary Metaproteomes without Genomic Information**; Hiroshi Nishida[1]; Akiyasu C. Yoshizawa[1]; Tsuyoshi Tabata[1]; Naoyuki Sugiyama[1]; Shujiro Okuda[2]; Yasushi Ishihama[1]; [1]*Graduate School of Pharmaceutical Sciences Kyoto University, Kyoto, Japan;* [2]*Niigata University Graduate School of Medical and Dental Sciences, Niigata, Japan*

MP 409 **Development of Custom Peptide MS/MS Analysis Software for Use in a Regulated Environment**; Roger E Moore[1]; Denise A Keen[1]; Gabriel B Gugiu[1]; [1]*City of Hope, Duarte, CA*

MP 410 **The Curation of Transcriptomic Data for Use as a Proxy Protein Database for Unsequenced Tree Nuts**; Cary Pirone-davies[1]; Melinda A. McFarland[1]; Christine H. Parker[1]; Timothy R. Croley[1]; [1]*U.S. Food and Drug Administration, College Park, MD*

MP 411 **Parametric Model Selection Methods for Estimating Target and Decoy Distributions Using Mass Spectrum Characteristics**; Benjamin A. Stark[1]; Robert Smith[1]; [1]*University of Montana, Missoula, MT*

MP 412 **MetaMorpheus Multi-Protease Parsimony Significantly Improves Protein Inference in Bottom-Up Proteomics**; Rachel M. Miller[1]; Robert J. Millikin[1]; Connor V. Hoffmann[1]; Stefan K. Solntsev[1]; Gloria M. Sheynkman[2]; Michael R. Shortreed[1]; Lloyd M. Smith[1]; [1]*University of Wisconsin, Madison, WI;* [2]*Dana-Farber Cancer Institute, Boston, MA*

MP 413 **A Novel LC-MS Deep Learning Based Cancer Detection Program and Improvements with Retention Time Correction**; Yuichi Kokabu[1]; Yukihiro Fukamachi[1]; Yoriko Takahashi[1]; Yasuto Yokoi[1]; Masaya Ono[2]; [1]*MITSUI KNOWLEDGE INDUSTRY CO., LTD., Minato-ku, Japan;* [2]*National Cancer Center Research Institute, Chuo-ku, Japan*

MP 414 **Optimizing the Isolation Width in Orbitrap Instruments to Maximize the Number of Label-Free Quantified Peptides and Protein**; Carmen Paschke[1]; Waqas Nasir[1]; Kai Fritzemeier[1]; Rosa Rakownikow Jersie-Christensen[1]; Tabiwang N. Arrey[1]; David Horn[2]; Martin Zeller[1]; Romain Huguet[2]; Bernard Delanghe[3]; [1]*Thermo Fisher Scientific, Bremen, Germany;* [2]*ThermoFisher, San Jose, CA;* [3]*Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

MP 415 **An Automated Data Analysis Workflow for Intact and Sub-Unit Mass Analysis of Protein Reagents Using Different Mass Spectrometry Platforms**; Dylan Sorensen[1]; Han-Yin Yang[1]; St. John Skilton[2]; Eric Carlson[2]; Dhanashri Bagal[1]; [1]*Amgen, South San Francisco, CA;* [2]*Protein Metrics Inc., Cupertino, CA*

MP 416 **FragPipe: A Fast Proteomics Pipeline with MSFragger Search Engine at Heart**; Dmitry Avtonomov[1]; Andy T. Kong[1]; Felipe V. Leprevost[1]; Guo-Ci Teo[1]; Hui-Yin Chang[1]; Alexey I. Nesvizhskii[1]; [1]*University of Michigan, Ann Arbor, MI*

MP 417 **End-to-End Integration of Known Variants and Modifications from PEFF into the Trans-Proteomic Pipeline for Enriched MS/MS Sequence Determination**; Luis Mendoza[1]; Eric W Deutsch[1]; Jimmy K Eng[2]; Robert L Moritz[1]; [1]*Institute for Systems Biology, Seattle, WA;* [2]*University of Washington, Seattle, WA*

MP 418 **TOMAHTO - An API-enhanced, TMT-based, Targeted Protein Assay with Real-time Instrument Control**; Qing Yu[1]; Devin K Schweppe[1]; Jose Navarrete-Perea[1]; Christopher M. Rose[2]; Bhavin Patel[3]; John C Rogers[3]; Steven P Gygi[1]; [1]*Harvard Medical School, Boston, MA;* [2]*Genentech, South San Francisco, CA;* [3]*ThermoFisher Scientific, Rockford, IL*

MP 419 **Model-Free SILAC Quantitation Yields Robust Reproducible Results**; David Chiang[1]; Patrick Chu[1]; *[1]Sage-N Research, Inc., Milpitas, CA*

MP 420 **gpGrouper: A Gene-Centric Peptide Grouping Procedure Accurately Distributes Shared Peptides Across Gene Products and Species**; Alexander Saltzman[1]; Bhoomi Bhatt[1]; Mei Leng[1]; Anna Malovannaya[1]; *[1]Baylor College of Medicine, Houston, TX*

MP 421 **Assessing the validity of protein inference on a large environmental metaproteomic dataset - ProteOMZ Expedition of the Central Pacific Ocean**; Jaclyn K. Saunders[1]; Matthew McIlvin[1]; Dawn Moran[1]; Noelle Held[1]; Chris Dupont[2]; Alyson Santoro[3]; Mak Saito[1]; *[1]Woods Hole Oceanographic Institution, Woods Hole, MA; [2]J. Craig Venter Institute, La Jolla, CA; [3]University of California, Santa Barbara, Santa Barbara, CA*

MP 422 **Propagating Uncertainty in Protein-Level Quantifications is Key to Robust Downstream Analysis of Bottom-Up Proteomics Data**; Alexander Phillips[1]; Ranjeet S Bhamber[2]; Anna Tierney[3]; Martin Rusilowicz[3]; Simon Maskell[1]; Simon Hubbard[3]; Andrew R Jones[1]; Richard Unwin[3]; Andrew W Dowsey[2]; *[1]University of Liverpool, Liverpool, United Kingdom; [2]University of Bristol, Bristol, United Kingdom; [3]University of Manchester, Manchester, United Kingdom*

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MP 423 **Automated Software for Enhanced Ion Mobility-Mass Spectrometry Analyses with Structures for Lossless Ion Manipulations**; Aivett Bilbao[1]; Joon-Yong Lee[1]; Bryson C. Gibbons[1]; Gabe Nagy[1]; Matthew E. Monroe[1]; Thomas O. Metz[1]; John C. Fjeldsted[2]; Yehia M. Ibrahim[1]; Richard D. Smith[1]; *[1]Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; [2]Agilent Technologies, Santa Clara, CA*

MP 424 **New Data Container Construct for Automated Processing of LC/UV/MS Data to Support High Throughput Chemistry**; Richard Lee[1]; Andrey Paramonov[1]; *[1]ACD/Labs, Toronto, ON*

MP 425 **The Web-Based Application for Exploring Isoform Specific Protein Expression Patterns in Mass Spectrometry Proteomics Data Repositories**; Han-Yin Yang[1]; Bradford W. Gibson[1]; *[1]Amgen Inc., South San Francisco, CA*

MP 426 **Systematic Evaluation of Cross-linked Peptide Search Engines**; Zhen-lin Chen[1]; Jia-Ming Meng[1]; Yong Cao[2]; Ji-Li Yin[1]; Run-Qian Fang[1]; Sheng-Bo Fan[1]; Chao Liu[1]; Wen-Feng Zeng[1]; Yue-He Ding[2]; Dan Tan[2]; Long Wu[1]; Wen-Jing Zhou[1]; Hao Chi[1]; Rui-Xiang Sun[2]; Meng-Qiu Dong[2]; Si-Min He[1]; *[1]Institute of Computing Technology, Chinese Academy of Sciences, Beijing, China; [2]National Institute of Biological Sciences, Beijing, China*

MP 427 **Populating a Vacuum Ultraviolet Spectroscopy Library Using Tandem GC/VUV-MS and Chemometric Deconvolution of Real-World Sample Data**; Shubhneet Warar[1]; Ian G. M. Anthony[2]; Christina A. Gaw[2]; Touradj Solouki[2]; *[1]Baylor Univeristy, Waco, TX; [2]Baylor University, Waco, TX*

MP 428 **triMS5 – A Novel Data Format for LC-IMS-MS Data Sets Providing Scalable Representation for Sparse Profile Data**; Jennifer Leclaire[1]; Thomas Kemmer[1]; Andreas Hildebrandt[1]; Stefan Tenzer[2]; *[1]University of Mainz, Mainz, Germany; [2]University Medical Center Mainz, Mainz, Germany*

MP 429 **A Platform Approach to Managing Developability and Manufacturability Assessments of Biotherapeutics**; Albert Van Wyk[1]; Joe Shambaugh[2]; John McCarter[2]; Aude Tartiere[3]; Christopher Smith[2]; Amanda Fitzgerald[2]; Cassandra Wigmore[4]; Peter Haberl[5]; *[1]Genedata Ltd, Cambridge, United Kingdom; [2]Genedata, Inc., Lexington, MA; [3]Genedata, Inc., San Francisco, CA; [4]Genedata AG, Basel, Switzerland; [5]Genedata GmbH, Munich, Germany*

MP 430 **Customizable Quality Control Metrics and Notifications with Panorama, AutoQC, and Skyline**; Josh Eckels[1]; Vagisha Sharma[2]; Marty Pradere[1]; Ankur Juneja[1]; Angelica Omaiye[1]; Cory Nathe[1]; Sweta Jewargikar[1]; Michael J MacCoss[2]; Brendan X MacLean[2]; *[1]LabKey, San Diego, CA; [2]University of Washington, Seattle, WA*

MP 431 **ASMS 2019 Abstract - Audit Logs to Enforce Document Integrity in Skyline and Panorama**; Tobias Rohde[1]; Rita Chupalov[1]; Nicholas Shulman[1]; Josh Eckels[2]; Brian S Pratt[1]; Michael J MacCoss[1]; Brendan X MacLean[1]; *[1]University of Washington, Seattle, WA; [2]LabKey, San Diego, CA*

MP 432 **MZView: Web-based Free Software for LC-MS Data Visualization**; Lin Wu[1]; Bin Ma[1]; *[1]University of Waterloo, Waterloo, ON*

MP 433 **On-Demand Construction of HRAM MSn Spectral Libraries: Where Acquisition Meets Curation**; Jakub Mezey[1]; Samuel Benkovič[1]; Melissa Montoya[2]; Tim Stratton[2]; Robert Mistrik[1]; Michal Raab[1]; *[1]HighChem, Bratislava, Slovakia; [2]Thermo Fisher Scientific, Austin, Texas*

MP 434 **Implementing a Generic Scripting Node to a Standard Proteomics Workflow Processing Software**; Frank Berg[1]; Kai Fritzemeier[1]; Carmen Paschke[1]; Torsten Ueckert[1]; David Horn[2]; Bernard Delanghe[1]; *[1]Thermo Fisher Scientific, Bremen, Germany; [2]ThermoFisher, San Jose, CA*

MP 435 **Simple Interface Web Application for Biomaker Validation**; Jaenyeon Kim[1]; Hyunsoo Kim[2]; Injoon Yeo[3]; Areum Sohn[2]; Youngsoo Kim[2, 3, 4]; *[1]Seoul National University, Seoul, South Korea; [2]Seoul National University College of Medicine, Seoul, South Korea; [3]Seoul national university, Seoul, South Korea; [4]Seoul National University Hospital, Seoul, South Korea*

MP 436 **mzMLb: A PSI Standards Compatible Binary Mass Spectrometry Data Format for Efficient Read/Write Speed and Storage Space Requirements**; Ranjeet S Bhamber[1]; Andris Jankevics[2]; Andy Jones[3]; Andrew Dowsey[1]; *[1]University of Bristol, Bristol, United Kingdom; [2]University of Birmingham, Birmingham, United Kingdom; [3]University of Liverpool, Liverpool, United Kingdom*

MP 437 **The implementation of MSFragger and Philosopher/ PeptideProphet nodes in Proteome Discoverer**; Hui-Yin Chang[1]; Andy T. Kong[1]; Felipe V. Leprevost[1]; Guo Ci Teo[1]; Venkatesha Basrur[1]; Alexey I. Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, MI*

MP 438 **Proteomics Standards Initiative Extended FASTA Format (PEFF)**; Pierre-Alain Binz[1]; Jim Shofstahl[2]; Juan Antonio Vizcaino[3]; Harald Barsnes[4]; Robert Chalkley[5]; Gerben Menschaert[6]; Emanuele Alpi[3]; Karl Clauser[7]; Jimmy K Eng[8]; Lydie Lane[9]; Sean seymour[10]; Gerhard Mayer[11]; Martin Eisenacher[11]; Yasset Perez-Riverol[3]; Eugene Kapp[12]; Luis Mendoza[13]; Peter R. Baker[5]; Eric Deutsch[13]; *[1]CHUV Centre Hospitalier Universitaire Vaudois, Lausanne, Switzerland; [2]Thermo Fisher Scientific, San Jose, California; [3]EMBL-EBI, Hinxton, United Kingdom; [4]University of Bergen, Bergen, Norway; [5]UCSF, San Francisco, CA; [6]Ghent University, Gent, Belgium; [7]Broad Institute of MIT and Harvard, Cambridge; [8]University of Washington, Seattle, WA; [9]SIB Swiss Institute of Bioinformatics, Geneva, Switzerland; [10]Seymour Data Science, San Francisco, California; [11]Ruhr University Bochum, Bochum, Germany; [12]University of Melbourne, Melbourne, Australia; [13]Institute for Systems Biology, Seattle, WA*

MP 439 **Proteomics Standards Initiative (PSI) Universal Spectrum Identifier (USI)**; Eric Deutsch[1]; Juan Antonio Vizcaino[2]; Yasset Perez-Riverol[2]; Jeremy Carver[3]; Benjamin Pullman[3]; Shin Kawano[4]; Zhi Sun[1]; Luis Mendoza[1]; Pierre-Alain Binz[5]; Gerben Menschaert[6]; Nuno Bandeira[3]; *[1]Institute for Systems Biology, Seattle, WA; [2]EMBL-EBI, Hinxton, United Kingdom; [3]UCSD, La Jolla, CA; [4]Database Center for Life Science, Kashiwa, Japan; [5]CHUV Centre Hospitalier Universitaire Vaudois, Lausanne, Switzerland; [6]Ghent University, Gent, Belgium*

MP 440 **Repository Scale MS1 Data Processing and Analysis Across Different LC-MS Methods**; Christine M Aceves[1]; Alan K Jarmusch[1]; Mingxun Wang[1]; Fernando Vargas[1]; Pieter Dorrestein[1]; *[1]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA*

MP 441 **Panorama Public: ProteomeXchange and Cloud Storage Integration**; Vagisha Sharma[1]; Brian Connolly[1]; Josh Eckels[2]; Dave Bradlee[2]; Angelica Omaiye[2]; Trey Chadick[2]; Michael J MacCoss[1]; Brendan X MacLean[1]; *[1]University of Washington, Seattle, WA; [2]LabKey, San Diego, CA*

MP 442 **ProteinExplorer: A Repository-Scale Resource for Exploration of Protein Detection in Public Mass Spectrometry Data Sets**; Benjamin Pullman[1]; Julie S Wertz[1]; Jeremy Carver[1]; Nuno Bandeira[1]; *[1]UC San Diego, La Jolla, CA*

MP 443 **proteoQ: An R Package for Versatile Integration of Bioinformatics with Multiplex, High-precision Proteomics**; Qiang Zhang[1]; R Reid Townsend[2]; *[1]Washington University School of Medicine, St. Louis, MO; [2]Washington University, School of Medicine, St. Louis, MO*

MP 444 **LipidXplorer Web: An Online Tool for Simplified and Streamlined Lipid Identification by Shotgun Lipidomics**; Eduardo Jacobo Miranda Ackerman[1]; Nils Hoffmann[2]; Oskar Knittelfelder[1]; Kai Schuhmann[1]; Robert Ahrends[2]; Andrej Shevchenko[1]; *[1]Max Plank Institute for Molecular Cell Biology and Genetics, Dresden, Germany; [2]Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany*

MP 445 **MassIVE: Converting Terabytes of Raw Public Data into Reusable Community Knowledge**; Jeremy Carver[1]; Mingxun Wang[1]; Benjamin Pullman[1]; Julie S Wertz[1]; Nuno Bandeira[1]; *[1]UCSD, La Jolla, CA*

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MP 446 **Small Molecule Detection from Biofluids using an Automated Plate-Based Paper Spray System**; Nicholas Manicke[1]; Greta J. Ren[1]; Cornelia Boeser[2]; Neloni Wijeratne[2]; *[1]IUPUI Department of Chemistry & Chemical Biology, Indianapolis, IN; [2]ThermoFisher, San Jose, CA*

MP 447 **Analysis of PFASs in Environmental Waters by DART-MS with Coated Dip-it Sampling in Minutes**; Robert Cody[1]; Simin D. Maleknia[2]; *[1]JEOL USA, Inc., Peabody, MA; [2]University of Technology Sydney, Sydney, Australia*

MP 448 **Vapor Assisted Ionization Enhancement in An Enclosed Nano-ESI Source**; Yixin Zhu[1]; Georgia Dolios[2]; Fangjun Wang[3]; Rong Wang[2]; Kai Tang[1]; *[1]Zhejiang Haochuang Biotech Co. Ltd., Hangzhou, China; [2]Icahn School of Medicine at Mount Sinai, New York, NY; [3]Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China*

MP 449 **Enhancement of Molecular Coverage by Solvent Gradient Electrospray Ionization Using Theta-Glass Capillary Emitters with Laser Ablation Mass Spectrometry**; Sara K Mattson[1]; Sylwia A Stopka[1]; Akos Vertes[1]; *[1]George Washington University, Washington, DC*

MP 450 **Modelling and Experimental Progress towards the Fabrication of Robust Constant-Bore Emitters and their Evaluation on a Novel Electrospray Test Device**; Kyle Bachus[1]; Joe Giddings[2]; Herbert Foo[1]; Heike Ebendorff-Heidepriem[2, 3]; Yvonne Stokes[2]; Andrew A Gooley[1]; *[1]Trajan Scientific and Medical, Ringwood, Australia; [2]University of Adelaide, Adelaide, Australia; [3]Institute for Photonics and Advanced Sensing, Adelaide, Australia*

MP 451 **Evaluation of Bare and Modified Copper Surfaces as Spray Initiators for Ambient Ionization**; Michael C. Godwin[1]; William D. Hoffmann[1]; *[1]Texas State University, San Marcos, TX*

MP 452 **Intra-well Imaging of Fluid Meniscus and Mass Spectra *via* Acoustic Mist Ionization Mass Spectrometry**; Eric Hall[1]; Lucien Ghislain[1]; Yi-wen Huang[1]; Sammy S Datwani[1]; *[1]Labcyte Inc., San Jose, CA*

MP 453 **Development of Novel Ion Source in a Portable Mass Spectrometer**; Yi-Shin Chen[1]; I-Chung Lu[1]; *[1]Department of Chemistry, National Chung Hsing University, Taichung City, Taiwan*

MP 454 **Acoustic-Droplet-Ejection to the Open-Port Probe Sampling Interface of MS (ADE-OPP-MS) - the Automated High-Throughput Bioanalysis Platform for Drug Discovery**; Chang Liu[1]; Hui Zhang[2]; Wenyi Hua[2]; Jianhua Liu[2]; David M Cox[1]; Thomas R. Covey[1]; *[1]SCIEX, Concord, ON; [2]Pfizer Inc., Groton, CT*

MP 455 **Direct Coupling of Magnetic Nanoparticles and Enhancement of Blade Spray Ionization Mass Spectrometry for Quantitation of Analytes in Complex Matrices**; Varoon Singh[1]; German Augusto Gomez Rios[1, 2]; Milaan Thirukumaran[1]; Daniel Rickert[1]; Janusz Pawliszyn[3]; *[1]University of Waterloo, Waterloo, ON; [2]Restek Corporation, Bellefonte, PA; [3]Univeristy of Waterloo, Waterloo, ON*

MP 456 **Comparison of Electrospray and Impactor Ionization (Unispray) Tandem Mass Spectrometry for the Analysis of Newborn Screening Biomakers**; Gyliann M Pena[1]; Timothy Lim[1]; Joanne Mei[1]; Konstantinos Petritis[1]; *[1]CDC, Atlanta, GA*

MP 457 **Establishing Better Laboratory Protocols for Desorption Ionization Using through Hole Alumina Membrane (DIUTHAME)**; Yasuhide Naito[1]; Masahiro Kotani[2]; Miu Takimoto[2]; Takayuki Ohmura[2]; *[1]GPI, Hamamatsu, Japan; [2]Hamamatsu Photonics K.K., Iwata, Japan*

MP 458 **Large-Area Triboelectric Nanogenerator Nanoelectrospray Ionization**; Marcos Bouza Areces[1, 2]; Yafeng Li[1]; Changsheng Wu[1]; Zhong Lin Wang[1, 3]; Facundo M. Fernandez[1, 2]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]Center for Chemical Evolution, Atlanta, GA; [3]Beijing Institute of Nanoenergy and Nanosystems, Chinese Academy of Sciences, Beijing, China*

MP 459 **Routine Absorption Mode FTMS Data Display with an Ethoxylated Anionic Detergent as a Dual-Role (Mass and Phase) Calibrant**; Daniel Cole[1]; Peifeng Hu[1]; *[1]Baxter Healthcare, Round Lake, IL*

MP 460 **Surface Effects in Droplet Chemistry Revealed by Transmission-Mode Liquid Desorption Electrospray Ionization**; Taghi Sahraeian[1]; Dmytro Kulyk[1]; Abraham K. Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH*

MP 461 **Liquid Injection Field Desorption Ionization in a Host EI/CI Source of a Time-of-Flight Mass Spectrometer**; Mathias Linden[1]; H. Bernhard Linden[1]; Jürgen H. Gross[2]; *[1]Linden CMS GmbH, Weyhe, Germany; [2]Institute of Organic Chemistry - Heidelberg University, Heidelberg, Germany*

MP 462 **Development of Vibrating Sharp-Edge Spray Ionization (VSSI) for Voltage-Free Mass Spectrometry Analysis**; Peng Li[1]; Xiaojun Li[2]; Nandhini Ranganathan[2]; Chong Li[2]; Stephen Valentine[2]; *[1]West Virginia University, Morgantown; [2]West Virginia University.C. Eugene Bennett Department of Chemistry, Morgantown, WV*

MP 463 **Open Port Probe for Rapid Analysis of Biological Samples: Application to Drug Discovery**; Stefan Thibodeaux; *Novartis, Cambridge, MA*

MP 464 **Next Generation Sample Introduction for High-Throughput Mass Spectrometry: Acoustic Droplet Ejection with an Open Port Probe**; Lucien Ghislain[1]; Chang Liu[2]; Hui Zhang[3]; Jianjua Liu[4]; Wenyi Hua[3]; Timothy Foley[3]; Don W. Arnold[5]; Thomas R. Covey[2]; Sammy S. Datwani[6]; *[1]Labcyte Inc, San Jose, CA; [2]SCIEX, Concord, ON; [3]Pfizer, Groton, CT; [4]Pfizer Inc., Groton, CT; [5]SCIEX, Redwood Shores, CA; [6]Labcyte Inc., San Jose, CA*

MP 465 **All in One Paper-Based Sample Preparation Integrated with Instant Immunocapture for Targeted Protein Analysis**; Øystein Skjærvø[1]; Trine Grønhaug Halvorsen[1]; Léon Reubsaet[1]; *[1]University of Oslo, Oslo, Norway*

MP 466 **Spray-Capillary: An Electrohydrodynamic Spray-Assisted Device for Quantitative Ultra-Low Volume Extraction**; Lushuang Huang[1]; Zhe Wang[1]; Si Wu[1]; *[1]University of Oklahoma, Norman, OK*

MP 467 **Regeneration of Dormant Soil Communities by Hydration: A New Platform for Assessing Soil Activity by Direct Real-Time Mass Spectrometry**; Karl Weitz[1]; Montana L. Smith[1]; Sheryl L. Bell[1]; Ljiljana Paša-Tolić[1]; Kirsten S Hofmockel[1]; Nicole M. Lock[2]; Malak M. Tfaily[1, 3]; Rosalie K. Chu[1]; Mary S. Lipton[1]; *[1]Battelle Pacific Northwest National Laboratories, Richland; [2]Shimadzu Scientific Instruments, Inc., Columbia, Maryland; [3]University of Arizona, Tucson, AZ*

MP 468 **A Microdroplet-Catalyzed Biginellireaction: Acceleration, Mechanisms and Separation of Isomers Using IMS-MS.**; Navneet sahota[1]; Deyaa I. AbuSalim[1]; Melinda L. Wang[1]; Tarick J. El-Baba[1]; Silas P. Cook[1]; David E. Clemmer[1]; *[1]Indiana University, Bloomington, IN*

MP 469 **Development of a 70kV Water Cluster Source for High-Resolution 3D Bio-Imaging**; Allen Bellew[1]; Sadia Sheraz née Rabbani[2]; Hua Tian[3]; Paul Blenkinsopp[1]; Peter J Cumpson[4]; Nicholas Winograd[5]; *[1]Ionoptika Limited, Chandler's Ford, United Kingdom; [2]Manchester Institute of Biotechnology, University of Manchester, United Kingdom; [3]Department of Chemistry, Pennsylvania State University, PA; [4]School of Mechanical and Systems Engineering, Newcastle University, United Kingdom; [5]Department of Chemistry, Pennsylvania State University, University Park, PA*

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MP 470 **Enrichment of Xenon Gas for Targeted Isotope Ratio Mass Spectrometry Utilizing a Digital Ion Trap**; Timothy Vazquez[1]; Colette Taylor[1]; Sean Williams[1]; Emily Smith[1]; Theresa Evans-Nguyen[1]; *[1]University of South Florida, Tampa, FL*

MP 471 **Back to Initial Ideas. Harmonized Kingdon Traps with Wire Internal Electrodes**; Eugene (evgeny) Nikolaev[1]; Oleg Kharybin[1]; Gleb Vladimirov[1]; Petr Borisovets[1]; Anton Lioznov[1]; Anastasia Fursova[1]; *[1]Skolkovo institute of science and technology, Moscow Region, Russian Federation*

MP 472 **Analytical Solution for the Electric Field Inside Dynamically Harmonized FT-ICR Cell**; Anton Lioznov[1]; Goekhan Baykut[2]; Eugene (evgeny) Nikolaev[1]; *[1]Skolkovo institute of science and technology, Moscow Region, Russian Federation; [2]Bruker Daltonik GmbH, Bremen, Germany*

MP 473 **A Novel Ion Guide Achieving High Transmission Efficiency under a Strong Gas Flow**; Masuyuki Sugiyama[1]; Hideki Hasegawa[1]; Yuichiro Hashimoto[2]; *[1]Hitachi, Ltd., Tokyo, Japan; [2]Hitachi high-technologies corporation, Hitachinaka, Japan*

MP 474 **Charge Detection Mass Spectrometry of Microparticles Using Printed Circuit Board Electrode Arrays**; Elaura Gustafson[1]; Halle V. Murray[1]; Yixin Song[1]; Jace Rozsa[1]; Shiuh-hua Chiang[1]; Aaron R. Hawkins[1]; Daniel E. Austin[1]; *[1]Brigham Young University, Provo, UT*

MP 475 **Optimization of the Ions Trajectories in a Dynamically Harmonized Fourier-Transform Ion Cyclotron Resonance Cell Using a Design of Experiments Strategy**; Julien Maillard[1, 2]; Justine Ferey[1]; Isabelle Schmitz-Afonso[1]; Soumeya Bekri[3]; Thomas Gautier[2]; Nathalie Carrasco[2]; Carlos Afonso[1]; Abdellah Tebani[3]; *[1]Université de Rouen, Laboratoire COBRA UMR 6014 & FR 3038, IRCOF, Mont St Aignan Cedex, France; [2]LATMOS/IPSL, Université Versailles St Quentin, UPMC Université Paris 06, CNRS, Guyancourt, France; [3]Department of Metabolic Biochemistry, Rouen University Hospital, Rouen, France*

MP 476 **Simulation of a Quadrupole Mass Filter Employing a Digital Waveform and Discontinuous Ion Introduction to Obtain High Resolution and Transmission**; David Langridge[1]; Martin Green[1]; Benjamin Jeffrey[2]; Robert Appleby[2]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]University of Manchester, Manchester, United Kingdom*

MP 477 **Evaluation of Two-Dimensional Mass Spectrometry Scans Using a Linear Ion Trap**; Lucas Szalwinski[1]; Dalton Snyder[2]; Zachary St. John[3]; Graham R. Cooks[1]; *[1]Purdue University, West Lafayette, IN; [2]Resource for Native Mass Spectrometry Guided Structural Biology, Columbus, OH; [3]The College of New Jersey Department of Chemistry, Ewing Township, New Jersey*

MP 478 **Application of CAN bus in Mass Spectrometer Design**; Ming Li[1]; Kai Li[1]; Xingbin Tang[1]; *[1]NCS Testing Technology Co., Ltd, Beijing, China*

MP 479 **Improvement of Electron Capture Efficiency in an RF Ion Trap by optimized Design of Magnetic Field**; Keqin Chen[1]; Goran Ristic[1]; Pavel Ryumin[1]; Bill Loyd[1]; Takashi Baba[1]; *[1]SCIEX, Concord, ON*

MP 480 **Advancement and Applications of Harmonic FTICR-MS Signals for Proteome Research**; Sung-Gun Park[1]; Jared P. Mohr[1]; Gordon Anderson[2]; James E. Bruce[1]; *[1]University of Washington, Seattle, WA; [2]GAA Custom Engineering, LLC, Benton, WA*

MP 481 **Detection of Bacteria Growth by ESI Ion Trap Mass Spectrometer**; Chun-Jen Hsiao[1]; Jung-Lee Lin[1]; Abdil Özdemir[2]; Chung-Hsuan Chen[1]; *[1]Genomics Research Center Academia Sinica, Taipei, Taiwan; [2]Department of Chemistry, Faculty of Arts and Sciences, Sakarya University, Esentepe, Turkey*

MP 482 **Characterization of Digital Mass Analysis in a Linear Trap without Resonant Ejection**; Margaret E. Reece[1]; Adam P. Huntley[1]; Peter T. A. Reilly[1]; *[1]Washington State University, Pullman, WA*

MP 483 **Methods to improve the Extraction Efficiency and Resolution of the Mass Selective Axial Ejection from a Linear Quadrupole Ion Trap**; Mircea Guna; *SCIEX, Concord, ON*

MP 484 **Design and Performance Improvement of an Ion Cooling Cell for a Quadrupole Mass Spectrometer**; Tsung-Chi Chen[1]; Eric C. Hemenway[1]; Paul H. Gregory[1]; Raman Mathur[1]; Hans Schweingruber[1]; Oleg Silivra[1]; Viatcheslav V. Kovtoun[1]; Michael Ugarov[1]; Jae C. Schwartz[1]; Alan E. Schoen[1]; *[1]ThermoFisher, San Jose, CA*

MP 485 **Improving the Coded Aperture Imaging in a Coded-Aperture Cycloidal Mass Spectrometer**; Raul Vyas[1]; Philip J. Herr[1]; Kathleen L Horvath[1]; Tanouir Aloui[1]; Matthew P. Kirley[1]; Charles B. Parker[1]; Adam D. Keil[2]; James B. Carlson[3]; Roger P. Sperline[4]; M Bonner Denton[4]; Brian R. Stoner[1]; Michael E. Gehm[1]; Jeffrey T Glass[1]; Jason J Amsden[1]; *[1]Duke University, Durham, NC; [2]Broadway*

Analytical, LLC, Monmouth, IL; [3]RTI International, Research Triangle Park, NC; [4]University of Arizona, Tucson, AZ

MP 486 **A Method to Determine the Mathematical Form of a Toroidal Trap Potential Starting with a Trap Geometry in SIMION® 8.1.**; Robert H. Jackson[1]; Stephen A. Lammert[2]; Atanu K. Mohanty[3]; Xiao Wang[4]; *[1]Instrumental Design Physics, Littleton, MA; [2]PerkinElmer Inc., American Fork, UT; [3]Indian Institute of Science, Bangalore, India; [4]PerkinElmer, American Fork, UT*

MP 487 **Increasing the Mass Range of Ion-Ion Reactions in a Quadrupole Ion Trap with Waveform Switching**; Kenneth W Lee[1]; Gregory S. Eakins[1]; Mark S. Carlsen[1]; Scott A. Mcluckey[1]; *[1]Purdue University, West Lafayette, IN*

MP 488 **Portable Ion Trap Mass Spectrometer with Paper Spray Ionization and Comprehensive Scan Modes for V-series Chemical Warfare Agent Identification**; Paul S Demond[1]; Dalton Snyder[2]; Ethan M McBride[3]; Carmany Daniel[1]; Elizabeth S Dhummakupt[3]; Phillip M Mach[3]; R. Graham Cooks[2]; Trevor Glaros[3]; *[1]Excet, Inc., Springfield, VA; [2]Purdue University, West Lafayette, IN; [3]ECBC, Aberdeen Proving Ground, Maryland*

MP 489 **Design and Performance of a Rotating Wall Analyzer for High-Throughput Ion Soft Landing**; Pei Su[1]; Hang Hu[1]; Don Gunaratne[2]; Julia Laskin[1]; *[1]Purdue University, West Lafayette, IN; [2]Pacific Northwest National Laboratory, Richland, WA*

MP 490 **Theoretical and Experimental Validation of High-Resolution Linear Time-of-Flight Mass Spectrometry**; Sheng-Wei Wu[1, 2]; Yu-Meng Ou[1, 2]; Yi-Hong Cai[1]; Chih-Hao Hsiao[1]; Cheng-Kai Jan[1]; Yi-Sheng Wang[1]; *[1]Academia Sinica, Taipei City, Taiwan; [2]National Taiwan University, Taipei, Taiwan*

MP 491 **Recent Development in Improving the Precision of Quantitative Analysis for Linear Ion Trap(LIT) and LIT-Orbitrap Tandem Mass Spectrometry**; Linfan Li[1]; Taoqing Wang[2]; Anyin Li[2]; Jae C Schwartz[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]University of New Hampshire, Durham, NH*

MP 492 **Application of a Triple Quadrupole MS with Acquisition Speed Improvements for Pesticide Analysis**; Harald Oser[1]; Michael Ugarov[2]; Qingyu Song[3]; Michael Konicek[1]; Claudia P.B. Martins[4]; Neloni Wijeratne[4]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, San Jose, California; [3]ThermoFisher Scientific, San Jose, CA; [4]ThermoFisher, San Jose, CA*

MP 493 **Negative Ions Detection with a Spaceflight-Designed Orbitrap-Based Mass Analyzer**; Barnabé Cherville[1]; Christelle Briois[1]; Laurent Thirkell[1]; Bertrand Gaubicher[1]; Fabrice Colin[1]; *[1]Laboratoire de Physique et de Chimie de l'Environnement et de l'Espace, Orléans, France*

MP 494 **High Throughput Charge Detection Mass Spectrometry**; Daniel Botamanenko[1]; Aaron R. Todd[1]; Martin F Jarrold[1]; *[1]Indiana University, Bloomington, IN*

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MP 495 **Quantitative Macrolipidomics of Human Whole Blood for the Discovery of Novel Biomarkers of omega-3 Polyunsaturate**; Juan Aristizabal-Henao[1]; Ningombam Sanjib Meitei[2]; Anja Pia Biltoft-Jensen[3]; Ken D. Stark[1]; *[1]University of Waterloo, Waterloo, ON; [2]PREMIER Biosoft, Palo Alto, CA; [3]Denmark Technical University, Lyngby, Denmark*

MP 496 **Untargeted Lipidomics Reveals Glycerolipid Compositional Changes in Fasted, Cold-Exposed MCAD KO Mice**; wenxuan zhang; *University Medical center Groningen, Groningen, Netherlands*

MP 497 **A Rapid Ion Mobility Enabled LC-MS Plasma Lipid Profiling Assay for Breast Cancer Biomarker Discovery**; Adam M King[1]; Jimmy Yuk[2]; Robert D Trengove[3]; Lauren G Mullin[2]; Paul D Rainville[2]; Giorgis Isaac[2]; Robert S Plumb[2]; Lee A Gethings[4]; Ian D Wilson[5]; *[1]Waters corporation, Wilmslow, United Kingdom; [2]Waters Corporation, Milford, MA; [3]Murdoch University, Perth, Australia; [4]Waters Corporation, Wilmslow, United Kingdom; [5]Imperial College, London, United Kingdom*

MP 498 **AcquireX Workflow Evaluation for Deciphering Lipidome Analysis of Lipids from Whole Insects Using Chromatography Based Methods with High-Resolution Orbitrap MSn**; Daniel Gachotte[1]; Yelena A Adelfinskaya[1]; Jeffrey Gilbert[1]; Reiko Kiyonami[2]; David Peake[2]; Yokoi Yasuto[3]; *[1]Corteva Agriscience, Indianapolis, IN; [2]Thermo Fisher Scientific, San Jose, CA; [3]Mitsui Knowledge Industry, Tokyo, Japan*

MP 499 **Red Blood Cell Membrane Fatty Acids in U. S. Blood Donors**; Carissa D. Powers[1]; David C. Scully[2]; Rosemary L. Schleicher[1]; *[1]Centers for Disease Control and Prevention, Atlanta, GA; [2]CDC Foundation, Atlanta, GA*

MP 500 **Tracking the Incorporation of Host Serum Lipids into the Membrane Lipids of *Staphylococcus aureus* with HILIC-IM-MS**; Kelly M. Hines[1]; Gloria Alvarado[2]; Craig Gatto[2]; Antje Pokorny[3]; Brian J. Wilkinson[2]; Libin Xu[1]; *[1]University of Washington, Seattle, WA; [2]Illinois state university, Normal, IL; [3]University of North Carolina Wilmington, Wilmington, NC*

MP 501 **Lipid Pool Coupling Analysis Based on Tandem Mass Spectrometric Data**; Jakob Koch[1]; Gregor Oemer[2]; Katrin Watschinger[3]; Sabrina Sailer[3]; Herbert Lindner[4]; Johannes Zschocke[2]; Markus A. Keller[2]; *[1]Division of Human Genetics, Medical Unversity of Innsbruck, Innsbruck, Austria; [2]Division of Human Genetics, Medical Unversity of Innsbruck, Innsbruck, Austria; [3]Division of Biological Chemistry, Biocenter, Medical University of Innsbruck, Innsbruck, Austria; [4]Division of Clinical Biochemistry, Biocenter, Medical University of Innsbruck, Innsbruck, Austria*

MP 502 **The Age of Dermal Fibroblasts in the Tumor Microenvironment Mediate Melanoma Cell Lipid Remodeling**; Aaron R. Goldman[1]; Gretchen M. Alicea[1, 2]; Delaine M. Zayas-Bazán[1, 3]; Hsin-Yao Tang[1]; Ashani T. Weeraratna[1]; David W. Speicher[1]; *[1]The Wistar Institute, Philadelphia, PA; [2]University of the Sciences, Philadelphia, PA; [3]University of Pennsylvania, Philadephia, PA*

MP 503 **Unconventional Synthesis of F-Series Prostaglandins from Lysate of *C. elegans* and their Identification by LC-MS/MS**; Ekta Tiwary[1]; Muhan Hu[1]; Landon S. Wilson[1]; Taylor F. Berryhill[1]; Michael A Miller[1]; Jeevan Prasain[1]; *[1]University of Alabama at Birmingham, Birmingham, AL*

MP 504 **Sphingolipid Phenotype of Adipocyte APP-Overexpressing Mice by LC/MS/MS and SCF/MS/MS**; Yu An[1]; Sarah Olive[2]; Benjamin Figard[2]; Philipp E. Scherer[1]; Ruth Gordillo[1]; *[1]UTSouthwestern Medical Center, Dallas, TX; [2]Shimadzu Scientific Instruments, Inc., Columbia, MD*

MP 505 **A New Lipidomics Software Workflow Demonstrates Disrupted Lipogenesis Induced with Drug Treatment in Leukemia Cells**; Mark Sartain[1]; Genevieve Van de Bittner[1]; Xiangdong Li[1]; Jeremy Koelmel[2]; Adithya Murali[1]; Sarah Stow[1]; *[1]Agilent Technologies, Santa Clara, CA; [2]Department of Chemistry, University of Florida, Gainesville, FL*

MP 506 **Desorption Electrospray Ionization Coupled to High Field Asymmetric Ion Mobility Mass Spectrometry Imaging for Investigating Cardiolipin Aberrations in Brain Cancer**; Anna C Krieger[1]; Clara Feider[1]; J. Clay Goodman[2]; Livia S. Eberlin[1]; *[1]The University of Texas at Austin, Austin, TX; [2]Departments of Pathology & Immunology and Neurology, Houston, TX*

MP 507 **Lipid Profiling of Malaria Samples Using Orbitrap Velos Pro Mass Spectrometer with SimLipid Software**; Ningombam Sanjib Meitei[1, 2]; Himani Gupta[2]; Fatima

Rahlouni[3]; David J. Sullivan[4]; Vladimir Shulaev[3]; [1]*PREMIER Biosoft, Palo Alto,, CA;* [2]*PREMIER Biosoft, Indore, India;* [3]*University of North Texas, Denton, TX;* [4]*Bloomberg School of Public Health, Johns Hopkins University, Baltimore, MD*

MP 508 **Lipidomics Reveals Site-Specific and Circulatory Lipid Profile Dysregulation in Low Carbohydrate/High Protein Diet when Compared to Western Diet**; Shama Naz[1,2]; Lise Cougnaud[1,3]; Fabiana A. Marques[1,4]; Heng Jiang[5]; Olivia H. Koury[6]; Mathilde Triquigneaux[1]; Andreas Bergdahl[6]; Dajana Vuckovic[1,2]; [1]*Department of Chemistry and Biochemistry, Concordia University, Montréal, QC;* [2]*The Centre for Biological Applications of Mass Spectrometry (CBAMS), Concordia University, Montréal, QC;* [3]*Department of Pharmaceutical Science, University of Bordeaux, Bordeaux, France;* [4]*Institute of Chemistry, University of Sao Paulo, São Carlos, Brazil;* [5]*The Centre for Biological Applications of Mass Spectrometry (CBAMS),Concordia University, Montréal, QC;* [6]*Department of Health, Kinesiology and Applied Physiology, Concordia University, Montréal, QC*

MP 509 **A Comprehensive Profiling Method for Regulatory Lipid Mediators Using UPLC TimsTOF**; Jun Yang[1]; Xuejun Peng[2]; Debin Wan[1]; Bruce D Hammock[1]; [1]*Department of Entomology and Nematology, University of California, Davis, Davis, CA;* [2]*Bruker Daltonics Inc., San Jose, CA*

MP 510 **MRM-Profiling as an Analytical Strategy to Perform the Analysis of Lipids in Extracellular Vesicles**; Madison E. Edwards[1]; Thomas De Luca[2]; Christina R. Ferreira[1]; Tiago J. P. Sobreira[1]; Eric A. Benson[2]; R. Graham Cooks[1]; [1]*Purdue University, West Lafayette, IN;* [2]*Indiana University School of Medicine, Indianapolis, Indiana*

MP 511 **Untargeted Lipidomic Profiling of Bis(monoacylglycero) phosphate Lipids in Cancer Cells and Tumor Tissues Point to Transformation Specific Regulation of Acyl Chains**; Megan Showalter[1]; Anastasia Berg[2]; Michael Sa[1]; Hiroshi Tsugawa[3]; Tobias Kind[1]; Kermit Carraway, III[2]; Oliver Fiehn[1]; [1]*UC Davis West Coast Metabolomics Center, Davis, CA;* [2]*Department of Biochemistry and Molecular Medicine UC Davis, Sacramento, CA;* [3]*RIKEN Center for Sustainable Resource Science, Wako, Japan*

MP 512 **Lipids is the Promising Biomarker to Classify HCC Cell Lines' Subtype Using SALDI-MS**; Tao Wang[1]; Jianmin Wu[1]; [1]*Zhejiang University, Hangzhou, China*

MP 513 **Comprehensive LC-MS Lipidomic Analysis of Viral and Plasma Lipid Alterations in SIV-Infected Rhesus Macaques Treated with and without Antiretroviral Agents**; Yong Jiang[1]; Sijia Tao[1]; Christina Gavegnano[1]; Ruby R Kleinbard[1]; Raymond F Schinazi[1]; [1]*Center for AIDS Research, Department of Pediatrics, Emory University, Atlanta, GA*

MP 514 **Lipidomic Analysis of IKE-Induced Ferroptosis in Lymphoma Mouse Model**; Fereshteh Zandkarimi[1,2]; Yan Zhang[3]; Hui Tan[3]; Jacob D. Daniels[4]; Hengrui Liu[3]; Lewis M. Brown[1,2]; Brent R Stockwell[1,3]; [1]*Department of Biological Sciences, Columbia University, New York, NY;* [2]*Quantitative Proteomics and Metabolomics Center, New York, NY;* [3]*Department of Chemistry, Columbia University, New york, NY;* [4]*Department of Pharmacology,Columbia University Medical Center, New York, NY*

MP 515 **Stools Lipid Profiling by HILIC LC-MS/MS – A Step Forward to a Non-Invasive Diagnostic of Diseases**; Justine Hustin[1]; Raphaël La Rocca[1]; Johann Far[1]; Delphine Debois[2]; Edwin De Pauw[1]; Gauthier Eppe[1]; Loïc Quinton[1]; [1]*University of Liege, MS Lab - GIGA, MolSys Research Unit, Liege, Belgium;* [2]*ZenTech S.A., Liege, Belgium*

MP 516 **Untargeted Lipidomics Analysis Reveals Effect of Abomasal Omega-3 Fatty Acid Infusion on Bovine Lipidome**; William Myers[1]; Eduardo Rico[1]; Joseph W McFadden[1]; Maria Elena Diaz Rubio[1]; Sheng Zhang[1]; [1]*Cornell University, Ithaca, NY*

MP 517 **Quantitative Analysis of Phospholipids and Triacylglycerol Lipids by Multiple Reaction Monitoring Profiling (MRM-Profiling)**; Zhuoer Xie[1]; Christina R. Ferreira[1]; Alessandra A. Vireque[2]; Tiago J. P. Sobreira[1]; R. Graham Cooks[1]; [1]*Purdue University, West Lafayette, IN;* [2]*Invitra, Assisted Reproductive Technologies Ltd., Ribeirão Preto, Brazil*

MP 518 **Separating and Profiling Phosphatidylcholines and Triglycerides from Single Lipid Droplet in HepG2 Cells by In-Tip Solvent Microextraction Mass Spectrometry**; Yaoyao Zhao[1]; Hitoshi Chiba[2]; Shu-Ping Hui[3]; [1]*Hokkaido University, Sapporo, Japan;* [2]*Sapporo University of Health Sciences, Sapporo, Japan;* [3]*Hokkaido University, Sapporo, Japan*

MP 519 **Lipidomic Profiling of Pancreatic Cancer Extracellular Vesicles Reveals Unique Signatures**; Shivani Bansal[1]; Charles P. Hinzman[1]; Michael Girgis[1]; Giorgis Isaac[2]; Nyasha Munjoma[2]; Amrita K. Cheema[1]; [1]*Georgetown University Medical Center, Washington, DC;* [2]*Waters Corporation, Milford, MA*

MP 520 **Novel Findings in HILIC Based LC-MS/MS Methods for Targeted Lipidomics Profiling**; Goncalo Vale[1]; Sarah Martin[2]; Mackenzie Pearson[3]; Jeffery G. McDonald[1]; [1]*UT Southwestern, Dallas, TX;* [2]*Agios Pharmaceuticals, Cambridge, MA;* [3]*Sciex, Redwood City, CA*

MP 521 **Development and Deployment of a Lipidomics Platform for the Characterization of Lipid Composition Differences in Strains of *Bacillus subtilis***; David Reeves[1,2]; Suresh Poudel[3]; Robert L. Hettich[1,3]; [1]*University of Tennessee, Knoxville, TN;* [2]*Oak Ridge National Laboratory, Oak Ridge, TN;* [3]*Oak Ridge National Laboratory, Oak Ridge, Tennessee*

MP 522 **Separation and Detection Method for the Profiling of Glycosphingolipids Using Liquid Chromatography Fluorescence Mass Spectrometry (LC-FLD-MS)**; Bela Reiz[1]; Radhika Chakraberty[1,2]; Randy M. Whittal[1]; Christopher W. Cairo[1,2]; [1]*Department of Chemistry, University of Alberta, Edmonton, Alberta;* [2]*Alberta Glycomics Centre, Edmonton, Alberta*

MP 523 **Combination of Distinctive Features Allows Rapid and Reliable Brain Tumor Tissue Identification**; Anatoly Sorokin[1,2]; Stanislav Pekov[1,3]; Vsevolod Shurkhay[1,4]; Vasiliy Eliferov[1]; Konstantin Bocharov[1]; Veronika Storozhilova[1]; Igor Popov[1,3]; Alexander Potapov[4]; Eugene (evgeny) Nikolaev[5]; [1]*Moscow Institute of Physics and Technology (State University), Dolgoprudny, Russia;* [2]*Institute of Cell Biophysics RAS, Pushchino, Russia;* [3]*Institute for Energy Problems of Chemical Physics RAS, Moscow, Russia;* [4]*N. N. Burdenko Scientific Research Neurosurgery Institute, Moscow, Russia;* [5]*Skolkovo institute of science and technology, Moscow Region, Russian Federation*

MP 524 **Mapping the Lipid Transducers of Exercise in Rats and Human Subjects**; David Gaul[1]; Sam Moore[1]; Alexandra Coomes[2]; Collin Douglas[2]; Karyn Esser[2]; Neil Johannsen[3]; Kate Early[4]; [1]*Georgia Institute of Technology, Atlanta, GA;* [2]*University of Florida, Gainesville, FL;* [3]*Louisiana State University, Baton Rouge, LA;* [4]*Columbus State University, Columbus, GA*

MP 525 **Development of Phospholipids Profiling of Mouse Tissues by PRM and Quantitative MS1 Multiplexing**; Xiaorong Fu[1]; Goncalo Vale[2]; Jeffrey G. M. McDonald[1]; Matthew Mitsche[1]; [1]*UT Southwestern Medical Center, dallas, Texas;* [2]*University of Texas Southwestern Medical Center, dallas, Texas*

MP 526 **S6K2 Inhibition Causes Lipid Remodeling and Reduced Growth in NRAS Mutant Melanoma Cells**; Delaine M. Zayas-Bazán[1,2]; Aaron R. Goldman[2]; Yun Hao[2,3]; Hsin-Yi Chen[2]; Jessie Villanueva[2]; David W. Speicher[2]; [1]*University of Pennsylvania, PA, PA;* [2]*The Wistar Institute, Philadelphia, PA;* [3]*University of Pennsylvania, Philadelphia*



MP 527 **Rapid and Sensitive Characterization of FAHFA Lipids Using an Untargeted Lipidomics Approach**; Tong Shen[1]; Bryan Roberts[1]; Oliver Fiehn[1]; *[1]UC Davis West Coast Metabolomics Center, Davis, CA*

MP 528 **Mapping the Algal Lipidome to Expand the Biofuel and Bioproduct Portfolio**; Peter V. Shanta[1]; Steven M. Rowland[1]; Stefanie Van Wychen[1]; Tao Dong[1]; Lieve M. Laurens[1]; *[1]National Renewable Energy Laboratory, Golden, CO*

MP 529 **Effects of Various Temperature Related Storage Conditions on Human Plasma and Serum Lipid Profile**; Greg B Reis[1]; Jon Rees[1]; Zsuzsanna Kuklenyik[1]; *[1]Centers for Disease Control and Prevention, Atlanta, Georgia*

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MP 530 **MSI and LC-MS Reveals Alterations of Phosphoinositides in Niemann-Pick Disease, Type C1**; Koralege Praneeth Chandimal Pathmasiri[1]; Melissa R Pergande[1]; Fernando Tobias[1]; Stephanie M Cologna[1]; *[1]University of Illinois at Chicago, Chicago, IL*

MP 531 **Mass Spectrometric Assessment on the Biological Fate of Gemini Surfactants Used as Gene Delivery Agents**; Wei Jin[1]; Mays Al-Dulaymi[1]; Randy Purves[2]; Ildiko Badea[1]; Anas El-Aneed[1]; *[1]University of Saskatchewan, Saskatoon, SK; [2]Centre for Veterinary Drug Residues, Canadian Food Inspection Agency, Saskatoon, SK*

MP 532 **Ion Suppressing Contaminants Generated by Multiple Injections from the Same Sample Vial Negatively Impact Reverse Phase Based-Lipidomics Experiments**; Peter Benke[1]; Bo Burla[1]; Kim Ekroos[2]; Markus R Wenk[1]; Federico Torta[1]; *[1]National University of Singapore, Singapore, Singapore; [2]Lipidomics Consulting Ltd, Esbo, Finland*

MP 533 **High-Throughput, Comprehensive Lipid/Protein Composition and Particle Number Analysis of Lipoproteins in Normal and Dyslipidemic Patients**; John R. Barr[1]; Michael Stephen Gardner[1]; Zsuzsanna Kuklenyik[1]; David Schieltz[1]; Antony Lehtikoski[2]; Jennifer Kusovschi[1]; Jon Rees[1]; Christopher Toth[1]; Michael S. Andrews[1]; Bryan M. Parks[1]; James L Pirkle[1]; *[1]CDC, Atlanta, GA; [2]Battelle Memorial Institute at the Centers for Disease Control and Prevention, Atlanta, GA*

MP 534 **High-Throughput Targeted Lipidomics Analysis of Dihydroceramide Desaturase-1 (DES1) Knockout Mice**; Mackenzie Pearson[1]; Santosh Kapil[1]; Trevor S Tippets[2]; Scott A Summers[2]; *[1]Sciex, Redwood City, CA; [2]University of Utah, Salt Lake City, UT*

MP 535 **An Inhibitor of iPLA2γ, R-BEL, Prevents Lipid Mediator Generation in the Ileum and Leads to Radiomitigation after Total Body Irradiation.**; Vladimir Tyurin[1]; Yulia Tyurina[1]; Andrew Amoscato[1]; Louis J. Sparovero[1]; Michael Epperly[1]; Claudette St. Croix[1]; Alan Watson[1]; Simon Watkins[1]; Joel Greenberger[1]; Hulya Bayir[1]; Valerian Kagan[1]; *[1]University of Pittsburgh, Pittsburgh, PA*

MP 536 ***P. aeruginosa* Lipoxygenase (pLoxA) Generates Ferroptotic Cell Death Signals in Host Human Bronchial Epithelial Cells: LC/MS Study.**; Yulia Tyurina[1]; Dar Haider[1]; Vladimir Tyurin[1]; Andrew Amoscato[1]; Joseph Joseph[1]; Rama Mallampalli[2]; Hülya Bayır[1]; Valerian Kagan[1]; *[1]University of Pittsburgh, Pittsburgh, PA; [2]The Ohio State University, Columbus, OH*

MP 537 **A Rapid Quantitative Method for Analysis of Oxidation Products of Cholesteryl Linoleate, Total Cholesteryl Esters, and Free Cholesterol by LC-APCI-MS/MS**; Michael Gardner[1]; Jon Rees[2]; Gregory Reis[2]; Lisa G. McWilliams[2]; Zsuzsanna Kuklenyik[2]; John R. Barr[2]; *[1]Centers for Disease Control and Prevention, Atlanta, GA; [2]Centers for Disease Control and Prevention, Atlanta, Ga*

MP 538 **Improved High-Throughput Targeted Lipidomic Analysis with sMRM Pro Builder**; Santosh Kapil Kumar Gorti[1]; Mackenzie Pearson[2]; Sean seymour[3]; Christie Hunter[4]; Paul Baker[4]; *[1]SCIEX, Framingham, MA; [2]Sciex, Framingham, MA; [3]Seymour Data Science, San Francisco, California; [4]Sciex, Redwood City, CA*

MP 539 **Enhanced Quantification of LPA 18:1 in Plasma with Differential Mobility Separation Technology**; Cyrus Papan[1]; Joerg Dojahn[1]; Sean Wu[2]; *[1]SCIEX, Darmstadt, Germany; [2]Sciex, Framingham, MA*

MP 540 **Quantifying the Lipidome for Respiratory Disease: A Rapid and Comprehensive HILIC-Based Targeted Approach**; Giorgis Isaac[1]; Nyasha Munjoma[2]; Lee A Gethings[2]; Robert S Plumb[1]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Wilmslow, United Kingdom*

MP 541 **Identification and quantitation of Lysophosphatidic Acid Regioisomeric Species in Mouse Plasma**; Juan Aristizabal-Henao[1]; Maria Fernanda Fernandes[1]; Robin E Duncan[1]; Ken D. Stark[1]; *[1]University of Waterloo, Waterloo, ON*

MP 542 **Combinatorial Chemistry to Synthesize Glycerolipidomic Mixtures with an Arbitrary Number of Components of Known Concentration**; Tom Brenna[1]; Dong Hao Park[1]; *[1]University of Texas at Austin, Austin, TX*

MP 543 **Semi-targeted Profiling of Fatty Acids Using Picolylamide Derivatization and C30 Reverse Phase Chromatography Coupled with High Resolution Tandem Mass Spectrometry**; Lucas Veillon[1]; Marc O. Warmoes[1]; Philip L Lorenzi[1]; John N Weinstein[1]; *[1]MD Anderson Cancer Center, Houston, TX*

MP 544 **Ganglioside Lipidomics in Human Dried Blood Spots Utilizing micro-LC/MS and MS/MS**; Asoka Ranasinghe[1]; Celia D'Arienzo[2]; Timothy Olah[2]; *[1]Bristol-Myers Squibb Company, Princeton, NJ; [2]Bristol-Myers Squibb Co., Princeton, NJ*

MP 545 **Dual Mass Spectrometry as a Tool to Improve Annotation and Quantification in Targeted Plasma Lipidomics**; Liang Gao[1]; Amaury Cazenave-Gassiot[2]; Bo Burla[1]; Markus R Wenk[3]; Federico Torta[3]; *[1]Singapore Lipidomics Incubator (SLING), Life Sciences Institute, National University of Singapore, Singapore, Singapore; [2]Department of Biochemistry, Yong Loo Lin School of Medicine, National University of Singapore, Singapore, Singapore; [3]Department of Biochemistry, Yong Loo Lin School of Medicine, National University of Singapore, Singapore, Singapore, Singapore*

MP 546 **Comprehensive Metabolic Profiling of Eicosanoids and Related Fatty Acids of Serum or Plasma by a Widely Targeted LC-MS/MS**; Masaki Yamada[1]; Huan Lin[1]; Takanari Hattori[1]; *[1]Shimadzu corp., Kyoto, Japan*

MP 547 **FIA-HRMS-Based Lipidomics Method: Comparing Measured Lipid Concentration Calculated Using Parent Molecular Ion Abundance Versus Sum of Product Ions Abundances**; Alexander Triebl[1]; Federico Torta[1]; Himani Gupta[2]; Ningombam Sanjib Meitei[2,3]; Rupanjan Goswami[2]; *[1]Singapore Lipidomics Incubator (SLING), Department of Biochemistry, YLL School of Medicine, National University of Singapore, Singapore; [2]PREMIER Biosoft, Indore, India; [3]PREMIER Biosoft, Palo Alto, CA*

MP 548 **Alteration of Lipidome Due to Vitamin B12 Deficiency**; Akash Kumar Bhaskar[1,2]; Khusbhoo Adlakha[1]; Salwa Naushin[1,2]; Arjun Ray[1]; Praveen Singh[1,2]; Monu Kumar[1]; Akanksha Singh[3]; Dipankar Malakar[3]; Christie Hunter[4]; Shantanu Sengupta[1,2]; *[1]CSIR-Institute of Genomics and Integrative Biology, New Delhi, India; [2]Academy of Scientific & Innovative Research, New Delhi, India; [3]SCIEX, Gurgaon, India; [4]Sciex, Redwood City, CA*

MP 549 **Analysis of Fatty Acids in GEMM Lymphatic Tumors with Mass Spectrometry: GC-MS Versus LC-MS**; Min Liu[1]; Jayden Cline[1]; Kristen E.N. Scott[1]; David C. Koomen[1]; John M. Koomen[1]; John L. Cleveland[1]; *[1]Moffitt Cancer Center, Tampa, FL*

MP 550 **Steroid Analysis in Human Plasma: Comparative Evaluation of Sorbent-Based Platforms for Phospholipid Removal**; Karolina M. Krasinska[1]; Allis S. Chien[1]; [1]*SUMS, Stanford University, Stanford, CA*

MP 551 **Fast Supercritical Fluid Chromatography Separation and Shotgun Lipidomics with High Resolution Mass Spectrometry for the Study of Breast Cancer Metastasis**; Sheher Mohsin[1]; Ningombam Sanjib Meitei[2]; Peter Siegel[3]; Daina Avizonis[4]; Gaelle Bridon[5]; [1]*Agilent Technologies, Schaumburg, IL;* [2]*PREMIER Biosoft, Indore, India;* [3]*Goodman Cancer Research Centre, Montreal, QC;* [4]*Goodman Cancer Research Centre, Quebec, Montreal, Canada;* [5]*Agilent Technologies, Inc., Wilmington, DE*

MP 552 **Analysis, Re-Analysis, and Quantitative Comparison of Lipidomics Using 13C-Labeled Cultures for Internal Standardization.**; Peining Xu[1]; Joyce Liu[2]; Sophie Trefely[1,2]; Clementina Mesaros[3]; Kathryn E. Wellen[2]; Nathaniel W Snyder[1]; [1]*Drexel University, Philadelphia, PA;* [2]*University of Pennsylvania, Philadelphia, PA;* [3]*University of Pennsylvania, Philadephia, PA*

MP 553 **Stable Isotope Labeling to Study Synaptamide Biosynthesis in Neuronal Cell Culture**; Karl R Kevala[1]; Michel Lagarde[2]; Arthur Spector[1]; Hee-Yong Kim[1]; [1]*NIAAA/ NIH, Rockville, MD;* [2]*Universite de Lyon, INSA, Lyon, France*

MP 554 ***in vivo* Measurement of Oxylipins in Rat Brain Using Solid-Phase Microextraction and LC-MS**; Alexander Napylov[1]; Nathaly Reyes Garces[2]; Mariola Olkowicz[2]; Sofia Lendor[2]; Ezel Boyaci[2]; German Gomez-Rios[2]; Cian Monnin[1]; Mustansir Diwan[3]; Barbara Bojko[2]; Clement Hamani[3]; Janusz Pawliszyn[2]; Dajana Vuckovic[4]; [1]*Concordia University, Montreal, Qc;* [2]*University of Waterloo, Waterloo;* [3]*Sunnybrook Health Sciences Centre, Toronto, ON;* [4]*Concordia University, Montreal, QC*

MP 555 **A Comparative Lipidomic Analysis between 2D and 3D Cell Culture of Adipocytes Derived from Mouse Primary Cell**; Jonghyun Kim[1]; Kyoung-Jin Choi[2]; Sung Bum Park[2]; Yoon-Ju Na[3]; Ki Young Kim[2]; Tae-Young Kim[1]; [1]*Gwangju Institute of Science & Technology, Gwangju, South Korea;* [2]*Therapeutics & Biotechnology Division, Korea Research Institute of Chemical Technology, Daejeon, South Korea;* [3]*Department of New Drug Discovery and Development, Chungnam National University, Daejeon, South Korea*

MP 556 **Comparison of Various Orthogonal Instrumental Approaches to Lipidomics Analysis of Human Blood**; Ken Riedl[1]; Ella Lin[1]; Kiran Boyinepally[1]; Ewy Mathe[1]; [1]*The Ohio State University, Columbus, OH*

MP 557 **Machine Learning Perspectives on Region of Interest Identification and Analysis in DESI Spectrometry**; Austin Ahlstrom[1]; John C Price[2]; [1]*Brigham Young University, Provo, UT;* [2]*Brigham Young University, Provo, Utah*

MP 558 **Stable Isotope Labeling by Permethylation and Reversed-Phase LC/MS for Relative Quantification of Intact Neutral Glycolipids in Mammalian Cells**; Rodell Barrientos[1,2]; Qibin Zhang[1,2]; [1]*Department of Chemistry and Biochemistry, University of North Carolina at Greensboro, Greensboro, NC;* [2]*UNCG Center for Translational Biomedical Research, Kannapolis, NC*

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MP 559 **THE SPECTRUM FACTORY: A New Workflow for the Creation of Libraries of Unknown Mass Spectra from Known Precursor Compounds**; John M. Halket[1]; Anna M. Caldwell[2]; W. Gary Mallard[3]; Stephen E. Stein[3]; [1]*King's College London, London, United Kingdom;* [2]*King's College London, London, United Kingdom;* [3]*NIST, Gaithersburg, MD*

MP 560 **Using Stable Isotope Labeling to Facilitate Unknown Metabolite Identification: A Case Study of Yeast Gene YNL010W**; Wenyun Lu[1]; Yifan Xu[2]; Joshua D. Rabinowitz[1]; [1]*Princeton University, Princeton, NJ;* [2]*DuPont Industrial Biosciences, Wilmington, DE*

MP 561 **Novel Deep Annotation Strategies for Non-Targeted Plant Metabolomics Based on High Resolution Mass Spectrometry**; Zaifang Li[1]; chunxia Zhao[1]; Xiuqiong Zhang[1]; Yueyi Xia[1]; Hua Zhang[1]; Xin Lu[1]; Guowang Xu[1]; [1]*CAS Key Laboratory of Separation Science for Analytical Chemistry, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China*

MP 562 **Identification of Metabolites from *Averrhoa camambola L.* Bark by Combination of Paper Spray & Electrospray Ionization Mass Spectrometry**; Syful Islam[1]; Md Badrul Alam[2]; Arif Ahmed[2]; Sunghwan Kim[2]; [1]*Department of Chemistry, Kyungpook National University, Daegu, South Korea;* [2]*Kyungpook National University, Daegu, South Korea*

MP 563 **Discovery of Unknown Metabolic Interactions of Microbiota & Human Host – Combining Novel Metabolomics and Chemical Biology Methodologies**; Daniel Globisch[1,2]; Louis P. Conway[1]; Mario S. P. Correia[1]; Caroline Ballet[1]; Neeraj Garg[1]; [1]*Uppsala University, Uppsala, Sweden;* [2]*SciLifeLab, Uppsala, Sweden*

MP 564 **Detecting Low Abundant Endogenous Cardiac Steroids from Biological Fluids Using Structure-Based MSn Approach On an OrbitrapTMTribridTM MS**; Reiko Kiyonami[1]; Michael Harrington[2]; Alfred Fonteh[2]; Roger Biringer[3]; Andreas Huhmer[1]; [1]*Thermo Fisher Scientific, San Jose, CA;* [2]*Huntington Medical Research Institutes, Pasadena, CA;* [3]*LECOM Bradenton, Bradenton, FL*

MP 565 **Magnetic Resonance Mass Spectrometry Profiling of Myxobacterial Extracts – Higher Resolution, Deeper Insights?**; Chantal Bader[1]; Patrick Haack[1]; Fabian Panter[1]; Matthias Witt[2]; Daniel Krug[1]; Rolf Müller[1]; [1]*Helmholtz-Institute for pharmaceutical research Saarland (HIPS), Saarbrücken, Germany;* [2]*Bruker Daltonik GmbH, Bremen, Germany*

MP 566 **Development of a *Caenorhabditis elegans* Reference Material for Long-Term LCMS Metabolomics Quality Control and Unknown Compound Identification**; Goncalo J. Gouveia[1]; Brianna M Garcia[2]; Emerson Ferreira Queiroz[3]; Franklin E. Leach III[4]; David L. Blum[1]; Jean-Luc Wolfender[3]; Lauren M. McIntyre[5]; I. Jonathan Amster[2]; Arthur S. Edison[1]; [1]*Department of Biochemistry and Molecular Biology, University of Georgia, Athens, GA;* [2]*Department of Chemistry, University of Georgia, Athens, GA;* [3]*School of Pharmaceutical Sciences, University of Geneva, Geneve, Switzerland;* [4]*Department of Environmental Health Science, University of Georgia, Athens, GA;* [5]*Department of Molecular Genetics and Microbiology, University of Florida, Gainsville, FL*

MP 567 **Novel Psychoactive Substances Detection Using a Novel Multi-Aspect Workflow Solutions**; Melissa Montoya[1]; Tim Stratton[1]; [1]*Thermo Fisher Scientific, Austin, Texas*

MP 568 **Electrochemical Simulation of Phase I Metabolism of Three Novel Cardiovascular Drugs Using UHPLC-MS/ MS**; Martin Eysberg[1]; Małgorzata Szultka-Młyńska[2]; Jean-Pierre Chervet[3]; [1]*Antec Scientific, Boston, MA 02108;* [2]*Department of Environmental Chemistry and Bioanalytics, Nicolaus Copernicus University, Torun, Poland;* [3]*Antec Scientific, Zoeterwoude, Netherlands*

MP 569 **Enabling Rapid and High-Confidence Metabolite Identification Using HILIC-QTOF Based MS/MS-RT library**; Shuang Zhao[1]; Wan Chan[1]; Ulrike Schweiger-Hufnagel[2]; Aiko Barsch[2]; Liang Li[1]; [1]*University of Alberta, Edmonton, AB;* [2]*Bruker Daltonik GmbH, Bremen, Germany*

MP 570 **A Complete Workflow for Improved Untargeted Metabolome Annotation and Identification Using Ultra High-Resolution Accurate Mass and LC-MSn Orbitrap-Based Mass Spectrometry**; David A. Peake[1]; Reiko Kiyonami[1]; Ioanna Ntai[1]; Amanda Souza[1]; Ralf Tautenhahn[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

MP 571 **Mass Spectrometry for Identification of Metabolites Secreted by Methamphetamine Treated Human Primary Macrophages**; Katarzyna Lech[1, 2]; Katarzyna Pawlak[1, 2]; Akou Vei[1]; Emma Harwood[1]; Spencer Marshall Jaquet[1]; Brenda Morsey[1]; Howard S. Fox[1]; Pawel Ciborowski[1]; *[1]University of Nebraska Medical Center, Omaha, NE; [2]Faculty of Chemistry, Warsaw University of Technology, Warsaw, Poland*

MP 572 **A Method of Calculating Retention Index of the Second Dimension Separation in Comprehensive Two-Dimensional Gas Chromatography Mass Spectrometry**; Md Aminul Islam Prodhan[1]; Ahmed A Sleman[1]; Xinmin Yin[1]; Pawel Lorkiewicz[1]; Seongho Kim[2]; Craig McClain[1]; Xiang Zhang[1]; *[1]University of Louisville, Louisville, KY; [2]Wayne State University, Detroit, MI*

MP 573 **Off-line fractionation of Complex Samples to Improve Depth-of-Coverage and Aid Compound Identification in Metabolomics**; Charles R Evans[1]; Brady G Anderson[1]; Maureen T Kachman[1]; *[1]University of Michigan, Ann Arbor, MI*

MP 574 **Comparison of Different Compound Spectral Libraries with DDA and DIA Analyzed Extracted Plasma for Metabolite Identification**; Robert Proos[1]; Khatereh Motamedchaboki[2]; Anthony Romanelli[1]; *[1]Sciex, Framingham, MA; [2]Sciex, Redwood City, CA*

MP 575 **IROA Approach Enabling Detection of Metabolites Whose Production is Initiated or Ceased in Response to Treatment**; Amy L. Lane[1]; Felice de Jong[2]; Chris Beecher[2]; *[1]University of North Florida, Jacksonville, FL; [2]IROA Technologies LLC, Bolton, MA*

MP 576 **CHO Cell Culture Media Profiling and Unknown Identification by Liquid Chromatography and Accurate Mass High Resolution Mass Spectrometry**; Richard Rogers[1]; Xuejun Peng[2]; Guillaume Tremintin[2]; *[1]Just Biotherapeutics, Seattle, WA; [2]Bruker Daltonics, San Jose, CA*

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MP 577 **Applications of a Novel Hydrolysis System for Deconvolution of Cyclotides on a Bead and Super Rapid Amino Acid Analyses**; Kiyoshi Nokihara[1]; Yuki Tominaga[1]; Takeshi Kasama[1]; Haruyuki Fujino[1]; Atsushi Kitagawa[1]; *[1]HiPep Laboratories, Kyoto, Japan*

MP 578 **Electron Transfer Dissociation of Highly Acidic peptides Following Enhanced Protonation Using Chromium(III) with Electrospray Ionization**; Surakshya Thapa[1]; Carolyn J. Cassady[1]; *[1]University of Alabama, Tuscaloosa, AL*

MP 579 **Proteogenomics-Assisted Identification of Novel Variants Peptides after p53 Loss in Wild-Type p53 Harboring Human Melanoma Cell Lines**; Satya Saxena[1, 2]; Mohd M Khan[3]; Jakub Faktor[4]; Nathan P Manes[5]; Sachin Kote[2]; Georges Bedran[2]; Javier Alfaro[2]; Aleksandra Nita-Lazar[5]; Borek Vojtesek[4]; Theodore Hupp[2, 6]; David R. Goodlett[2, 3]; *[1]Deurion LLC, Seattle, WA; [2]International Centre for Cancer Vaccine Science, University of Gdansk, Gdansk, Poland; [3]University of Maryland, Baltimore, MD; [4]RECAMO, Brno, Czech Republic; [5]NIH/NIAID, Bethesda, MD; [6]University of Edinburgh, Edinburgh, United Kingdom*

MP 580 **Analysis Platform for accurate amino acid sequencing combining with a benchtop MALDI-TOF MS and N-/C-terminal sequencing**; Nanami Sakashita[1]; Tomoko Kuriki[1]; Brian J. Field[2]; Yuzo Yamazaki[1]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Shimadzu Scientific Instruments, Inc., Columbia, MD*

MP 581 **Advances in Structural Elucidation Techniques for the Characterization of Cystine-Knot Peptides**; Sarah J. Robinson[1, 2]; Christopher M Crittenden[1]; *[1]Small Molecule Pharmaceutical Sciences, Genentech Inc., South San Francisco, CA; [2]Discovery Chemistry, Genentech Inc., South San Francisco, CA*

MP 582 **Characterization of Five Commonly Used Chymotrypsins**; Yunyun Zhu[1]; Alexander S. Herbert[2, 3, 4]; Joshua J Coon[2, 3, 4, 5]; *[1]University of Wisconsin-Madison, Madison, WI; [2]Genome Center of Wisconsin, Madison, WI; [3]Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; [4]Department of Biochemistry, University of Wisconsin,, Madison, WI; [5]Department of Chemistry, University of Wisconsin, Madison, WI*

MP 583 **Structural Characterization of Cyclic Peptides Using a Quadrupole Time-of-Flight Mass Spectrometer**; Toshiya Matsubara[1]; Yusuke Inohana[1]; Ichiro Hirano[1]; *[1]Shimadzu Corporation, Kyoto, Japan*

MP 584 **Investigating the Cleavage Capability of the Proteases LysN, LysArginase and Chymotrypsin in Complex, Biotinylated Samples**; Peter Schein[1]; Volkmar Gieselmann[1]; Marc Sylvester[1]; *[1]Institute of Biochemistry and Molecular Biology, Rheinische Friedrich-Wilhelms University of Bonn, Bonn, Germany*

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MP 585 **Multiplex Dimethylated Leucine (DiLeu) Isobaric Tags to Probe Neuropeptidomic Response to Copper Toxicity in the Blue Crab, *Callinectes sapidus***; Chris Sauer[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

MP 586 **Single Amino Acid Variant Discovery in 9 Panc-1 Cells**; Zhijing Tan[1]; Xinpei Yi[2]; Nicholas J. Carruthers[3]; Paul M. Stemmer[3]; David M. Lubman[4]; *[1]University of Michiagan, Ann Arbor, MI; [2]University of Chinese Academy of Sciences, Beijing, China; [3]Wayne State University, Detroit, Michigan; [4]University of Michigan, Ann Arbor, MI*

MP 587 **Capillary Zone Electrophoresis-Tandem Mass Spectrometry for Large-Scale Phosphoproteomics with over 11,000 Phosphopeptides IDs from the Colon Carcinoma HCT116 Cell Line**; Daoyang Chen[1]; Katelyn R. Ludwig[2]; Oleg V. Krokhin[3]; Vic Spicer[3]; Zhichang Yang[1]; Xiaojing Shen[1]; Amanda B. Hummon[4]; Liangliang Sun[1]; *[1]Department of Chemistry, Michigan State University, East Lansing, MI; [2]Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, IN; [3]Manitoba Centre for Proteomics and Systems Biology, University of Manitoba, Winnipeg, Manitoba; [4]Department of Chemistry and Biochemistry, Comprehensive Cancer Center, The Ohio State University, Columbus, OH*

MP 588 **Single Cell MALDI MS Neuropeptidomics of the Aplysia Californica**; Peter Andersen[1]; Thanh Do[2]; Stanislav S Rubakhin[1]; Jonathan V. Sweedler[1]; *[1]University of Illinois at Urbana Champaign, Urbana, IL; [2]University of Tennessee, Knoxville, TN*

MP 589 **Increasing the Analysis Depth of the HLA-Associated Peptide Repertoire by LC-MS/MS**; Chris D McGann[1]; Scott P Goulding[1]; Lia R Serrano[1]; Michael R Nelson[1]; Aman Makaju[2]; Jennifer G Abelin[1]; Terri A Addona[1]; *[1]Neon Therapeutics, Cambridge, MA; [2]Thermo Fisher Scientific, San Jose, CA*

MP 590 **Detection of Ultra-Low Abundance Epitopes by Parallel Reaction Monitoring (PRM)**; Jonas Förster[1, 2]; Nitya Mohan[1, 2]; Rebecca Köhler[1, 3]; Mogjib Salek[1, 3]; Angelika B. Riemer[1, 3]; *[1]German Cancer Research Center (DKFZ), Heidelberg, Germany; [2]Faculty of Biosciences, Heidelberg University, Heidelberg, Germany, Heidelberg, Germany; [3]Molecular Vaccine Design, German Center for Infection*

Research (DZIF), partner site Heidelberg, Heidelberg, Germany, Heidelberg, Germany

MP 591 **A Mass Spectrometry Based Platform for Differential Diagnostics of Hypertensive Pregnancy Complications *via* Urine Peptidome Profiling**; Alexey Kononikhin[1,2,3]; Victoria Sergeeva[3,4]; Natalia Starodubtseva[1,2]; Maria Indeykina[2,4]; Anna Bugrova[1,4]; Natalia V. Zakharova[4]; Vitaly Chagovets[1]; Igor Popov[1,2]; Vladimir Frankevich[1]; Eugene (evgeny) Nikolaev[5]; *[1]V. I. Kulakov National Medical Research Center for Obstetrics, Gynecology and Perinatology, Ministry of Healthcare of the Russian Federation, Moscow, Russia; [2]Moscow Institute of Physics and Technology (State University), Dolgoprudny, Russia; [3]V.L. Talrose Institute for Energy Problems of Chemical Physics, Russian Academy of Sciences, Moscow, Russia; [4]Emanuel Institute for Biochemical Physics, Russian Academy of Sciences, Moscow, Russia; [5]Skolkovo institute of science and technology, Moscow Region, Russian Federation*

MP 592 **Enhanced Detection of Short and Hydrophilic Peptides Fraction Using Porous Graphitic Carbon**; Susy Piovesana[1]; Carmela Maria Carmela Maria Montone[2]; Chiara Cavaliere[2]; Giorgia La Barbera[2]; Aldo Laganà[2]; Anna Laura Capriotti[2]; Carlo Crescenzi[3]; *[1]Department of Chemistry, Università di Roma "La Sapienza", Rome, Italy; [2]Department of Chemistry, Università di Roma "La Sapienza", Rome, Italy; [3]Salerno University, Fisciano (SA), Italy*

MP 593 **Intraspecific Comparison of the Venom Peptidome of *Conus purpurascens***; Meghan K. Grandal[1,2]; Mickelene F. Hoggard[1]; Frank Marí[1]; *[1]National Institute of Standards and Technology, Charleston, SC; [2]Medical University of South Carolina, Charleston, SC*

MP 594 **Optimized Mild Acid Elution and Sample Clean-Up of MHC Immunopeptides with Trapped Ion Mobility Spectrometry(tims)-TOF**; Teesha C Luehr[1]; Queenie Chan[1]; Leonard J Foster[1]; *[1]University of British Columbia, Vancouver, BC*

MP 595 **Quantitative Analysis of the Isoforms of the Master Iron Regulator Hepcidin in a Clinically Actionable Time Frame**; Robert Trengove[1,2]; Garth Maker[3,4]; *[1]Murdoch University, Murdoch, Australia; [2]Australian National Phenome Centre, Murdoch University, Perth, Australia; [3]Murdoch University, Perth, Australia; [4]Medical, Molecular and Forensic Sciences, Murdoch University, Murdoch, Australia*

MP 596 **Mass Spectrometry Based Immunopeptidomics - Accelerating the Development of Personalized Cancer Immunotherapy**; Michal Bassani-sternberg[1,2]; Markus Müller[3]; Florian Huber[1,2]; Brian Stevenson[3]; Julien Racle[4]; Justine Michaux[1,2]; Chloe Chong[1,2]; David Gfeller[4,5]; George Coukos[1,2]; *[1]Department of Oncology, University Hospital of Lausanne, Lausanne, Switzerland; [2]Ludwig Institute for Cancer Research, Lausanne, Switzerland; [3]Vital IT, Swiss Institute of Bioinformatics, Lausanne, Switzerland; [4]Department of Oncology, University of Lausanne, Lausanne, Switzerland; [5]Swiss Institute of Bioinformatics, Lausanne, Switzerland*

MP 597 **Characterization of Human Pancreatic Islet Peptidome Using Parallel Accumulation-Serial Fragmentation (PASEF) and Trapped Ion Mobility Spectrometry**; Elena V. Romanova[1]; Stanislav S Rubakhin[1]; David H. Mast[1]; Jonathan V. Sweedler[1]; *[1]University of Illinois at Urbana-Champaign, Urbana, IL*

MP 598 **Enrichment of Zinc Finger Proteins by IMAC**; Stephanie Miller Lehman[1]; Josue Baeza[1]; Geoffrey P. Dann[1]; Benjamin A Garcia[1]; *[1]University of Pennsylvania, Philadelphia, PA*

PHOSPHOPEPTIDES: ENRICHMENT METHODS
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MP 599 **A Novel Automated and Highly Selective Phosphopeptide Enrichment Strategy for Successful Phosphopeptide Identification and Phosphosite Localization**; Shuai Wu[1]; Kenneth Newton[1]; Linfeng Wu[1]; Jordy J. Hsiao[1]; Valery G. Voinov[2,3]; Joseph S. Beckman[2,3]; *[1]Agilent Technologies, Santa Clara, CA; [2]e-Msion Inc., Corvallis, OR; [3]Oregon State University, Corvallis, OR*

MP 600 **A Scalable Phosphopeptide Enrichment Strategy for Multiplexed Quantitative Phosphoproteomics**; Alison Erickson[1]; Brian Erickson[1]; Craig Braun[1]; Ryan Kunz[1]; *[1]IQ Proteomics LLC, Cambridge, MA*

MP 601 **Large Scale EasyPepTM MS Sample Preparation for Phosphopeptide Enrichment Workflows**; Amarjeet Flora[1]; Ryan D. Bomgarden[1]; Sergei Snovida[1]; Ashok Salunkhe[1]; John C. Rogers[1]; *[1]Thermo Fisher Scientific, Rockford, IL*

MP 602 **Development of Fully Automated and High-Throughput Workflow for Phosphoproteomics**; Stoyan Stoychev[1,2]; Ireshyn Govender[1]; Previn Naciker[1]; Sindisiwe Buthelezi[1]; Sipho Mamputha[1]; Isak Gerber[1,2]; Justin Jordaan[2]; *[1]CSIR, Pretoria, South Africa; [2]ReSyn BioSciences, Pretoria, South Africa*

MP 603 **Using Quantitative Phosphoproteomics to Understand Key Phosphorylation Signaling Pathways in HCT116 Cells after Chemotherapy Drug Treatment**; Brian T Mullis[1]; Lim Andrew Lee[2]; Rebekah J Woolsey[3]; David R Quilici[3]; Qian Wang[1]; *[1]University of South Carolina, Columbia, SC; [2]Integrated Micro-Chromatography Systems, Irmo, SC; [3]Mitch Hitchcock, Ph.D. Nevada Proteomics Center, Reno, NV*

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MP 604 **Discovering Putative Mode of Action of Plant Protection Genes Using Metabolomics**; Jan Hazebroek[1]; Teresa Harp[1]; Chris Vlahakis[1]; Leandro Perugini[1]; Girma Tabor[1]; *[1]Corteva Agriscience, Johnston, IA*

MP 605 **Drought Metabolomics of Susceptible and Tolerant Soybean Cultivars**; Kevin J. Zemaitis[1]; Philip Lindhorst[1]; Troy D. Wood[1]; *[1]University at Buffalo, Buffalo, NY*

MP 606 **Application of Data-Independent Acquisition Approach to Study the Proteome Dynamics of Plant Pathogenesis Responses**; Kai-ting Fan[1]; Kuo-Hsin Wang[1]; Wei-Hung Chang[1]; Jhih-Ci Yang Yang[1,2]; Ching-Fang Yeh[1]; Kai-Tan Cheng[1]; Sheng-Chi Hung[1,3]; Yet-Ran Chen[1]; *[1]Agricultural Biotechnology Research Center, Academia Sinica, Taipei, Taiwan; [2]National Chiao Tung University, Hsinchu, Taiwan; [3]Institute of Biotechnology, National Taiwan University, Taipei, Taiwan*

MP 607 **Using SWATH-MS to Understand Global Proteome Changes in Barley Lines with Reduced Storage Protein Synthesis**; Utpal Bose[1]; Keren Byrne[1]; Malcolm J. Blundell[2]; Crispin A. Howitt[2]; Michelle L. Colgrave[1]; *[1]Agriculture and Food, CSIRO, St Lucia, Australia; [2]Agriculture and Food, CSIRO, Canberra, Australia*

MP 608 **Dynamic Proteome Response of Different Rice Varieties to Drought Stress**; Sara Hamzelou[1]; Dana Pascovici[1]; Mehdi Mirzaei[1]; Ardeshir Amirkhani[1]; Matthew J. McKay[1]; Brian J. Atwell[1]; Paul A. Haynes[1]; *[1]Macquarie University, North Ryde, Australia*

MP 609 **Simple and High-Throughput Method for Plant Metabolites by PESI/MS/MS: First Application to Plant Metabolite Analysis and Agricultural Industry**; Ryota Harada[1]; Moeko Taki[1]; Yumi Hayashi[2,3]; Kei Zaitsu[2]; Katsuhiro Shiratake[1]; *[1]Laboratory of Horticultural Science, Graduate School of Bioagricultural Sciences, Nagoya University, Nagoya, Japan; [2]In Vivo Real-Time Omics Laboratory, Institute for Advanced Research, Nagoya*

University, Nagoya, Japan; [3]Pathophysiological Laboratory Sciences, Department of Radiological and Medical Laboratory Sciences, Nagoya University Graduate School of Medicine, Nagoya, Japan

MP 610 **Dissection of Flag Leaf Metabolic Shifts and Relationship with Those Occurring Simultaneously in Developing Seed by Application of Non-Targeted Metabolomics**; Chaoyang Hu[1]; Jianxin Shi[2]; Yue Song[3]; Shan-an Chan[4]; *[1]Ningbo University, Ningbo, China; [2]Shanghai Jiao Tong University, Shanghai, China; [3]Agilent Technologies, Shanghai, China; [4]Agilent Technologies, Taipei, Taiwan*

MP 611 **Metabolic Disturbance in the Beet Necrotic Yellow Vein Virus/Sugar Beet Pathosystem**; Fabio C. Chaves[1]; Kimberly M. Webb[2]; William M. Wintermantel[3]; Lisa M Wolfe[1]; Linxing Yao[1]; Corey D. Broeckling[1]; *[1]Proteomics and Metabolomics Facility of Colorado State University, Fort Collins, CO; [2]USDA-ARS, Soil Management and Sugar Beet Research Unit, Fort Collins, CO; [3]USDA-ARS, Crop Improvement and Protection Research Unit, Salinas, CA*

MP 612 **Phosphoproteomics Reveals the Downstream Phosphorylation Signaling Targets of the Lectin Receptor-Like Kinase PtLecRLK1 Involved in Plant *I Mycorrhizal symbiosis***; Him K Shrestha[1]; Paul Abraham[2]; Jin-Gui Chen[2]; Robert L. Hettich[2]; *[1]University of Tennessee, Knoxville, TN; [2]Oak Ridge National Laboratory, Oak Ridge, TN*

MP 613 **A Quantitative Strategy for Deep Coverage of the Algal Phosphoproteome**; Megan M. Ford[1]; Emily G. Werth[1]; Leslie M. Hicks[1]; *[1]University of North Carolina, Chapel Hill, NC*

MP 614 **Characterization and Identification of Di-Isodityrosine and Pulcherosine Cross-linkages Occurring in the Plant Cell Wall Extensin Scaffold**; Lawrie Gainey[1]; Steven D. Hartson[1]; Michelle English[2]; Marshall Bern[2]; Andrew J. Mort[1]; *[1]Oklahoma State University, Stillwater, OK; [2]Protein Metrics Inc., San Carlos, CA*

MP 615 **Enhancement of Nodule-Specific Cysteine-Rich Peptide Detection in Medicago truncatula by MALDI-MSI through Inclusion of a Simple Wash**; Caitlin Keller[1]; Nhu Q. Vu[1]; Bailey Kleven[1]; Sanhita Chakraborty[1]; Junko Maeda[1]; Dhileepkumar Jayaraman[1]; Michael R. Sussman[1]; Jean-Michel Ané[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

MP 616 **Elucidating Protein-Protein Interactions in *Chlamydomonas reinhardtii* Using Immunoprecipitation and Liquid Chromatography-Mass Spectrometry**; Anthony A Iannetta[1]; Leslie M Hicks[1]; *[1]University of North Carolina, Chapel Hill, NC*

MP 617 **Development and Characterization of IR-MALDESI Specifically for Mass Spectrometry Imaging of Plants**; Michael C Bagley[1]; Rika S Judd[1]; Anna N Stepanova[1]; Yogini S Jaiswal[2]; Måns Ekelöf[1]; Kenneth P Garrard[1]; Leonard L Williams[2]; Jose M Alonso[1]; De-Yu Xie[1]; David C Muddiman[1,3]; *[1]North Carolina State University, Raleigh, NC; [2]Center for Excellence in Post Harvest Technologies, North Carolina Agricultural and Technical State University, The North Carolina Research Campus, Kannapolis, North Carolina; [3]Molecular Education, Technology, and Research Innovation Center (METRIC), North Carolina State University, Raleigh, NC*

MP 618 **Proteoform Profiling of Canadian Breadwheat Glutenins Reveals Unexpected C-Terminal Tyrosine Truncation in Low Molecular Weight Glutenins**; Ray Bacala[1,2]; Katherine Cordova[1]; Helene Perreault[2]; Dave Hatcher[1]; *[1]Canadian Grain Commission, Winnipeg, MB; [2]Department of Chemistry, University of Manitoba, Winnipeg, MB*

MP 619 **The Metabolome of Early Season Sorghum Plant Tissue is Predictive of End of Season Biomass**; Amy M Sheflin[1]; Stephen Kresovich[2]; Ismail Dweikat[3]; Ellen Marsh[3]; Daniel Schachtman[3]; Jessica Prenni[1]; *[1]Colorado State University, Fort Collins, CO; [2]Clemson University, Clemson, SC; [3]University of Nebraska Lincoln, Lincoln, NE*

MP 620 **Proteomic Analysis of Translational Control of Gene Expression under Light Treatment in *Arabidopsis thaliana***; Yixiang Zhang[1,2]; Xuhong Yu[3]; Scott D. Michaels[3]; Jonathan C. Trinidad[1,2]; *[1]Department of Chemistry, Indiana University, Bloomington, IN; [2]Laboratory for Biological Mass Spectrometry, Indiana University, Bloomington, IN; [3]Department of Biology, Indiana University, Bloomington, IN*

MP 621 **Regulation at the Plant-Microbe Interface: Discovery and Characterization of Signaling Polypeptides Using High-Performance Tandem Mass Spectrometry**; Paul E. Abraham[1]; Suresh Poudel[1]; Anna Matthiadis[1]; Udaya Kalluri[1]; Robert L. Hettich[1]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN*

MP 622 **Profiling of Histone Acetylation and Methylation Marks Associated with Embryo and Aleurone Tissue-Specific Epigenetic Regulation of Seed Dormancy in Wheat**; Michelle Rampitsch[1]; Mei Huang[1]; Yao Zhen[1]; Nataša Radovanovic[1]; Wayne Xu[1]; Christof Rampitsch[1]; Natalia V. Bykova[1]; *[1]Agriculture and Agri-Food Canada, Morden, Manitoba*

MP 623 **Metabolome-Based Genome Wide Association Profiling of Innate Immunity in Rice**; Joshua Blakeslee[1]; Pengfei Bai[2]; Yun Li[1]; Matthew Bernier[2]; Guo-Liang Wang[2]; *[1]The Ohio State University, Wooster, OH; [2]The Ohio State University, Columbus, OH*

MP 624 **Molecular and Microbial Responses to Drought in Field-Grown Sorghum**; Kim K. Hixson[1]; Kristin M. Engbrecht[1]; Daniel J. Orton[1]; Kent J. Bloodsworth[1]; Aivett Bilbao[1]; Joon-Yong Lee[1]; Young-Mo Kim[1]; Jamie R. Nunez[1]; Bryan A. Stanfill[1]; Erika M. Zink[1]; Karl K. Weitz[1]; Ling Xu[2,3]; Pubudu P. Handakumbura[1]; Mary A. Madera[2]; Julie A. Sievert[4]; Joy Hollingsworth[4]; Ronald J. Moore[1]; Ryan S. Renslow[1]; Thomas O. Metz[1]; Ljiljana Pasa-Tolic[1]; Robert Hutmacher[5]; Jeffery A. Dahlberg[4]; Devin Coleman-Derr[2,3]; Peggy G. Lemaux[2]; Christer Jansson[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]University of California, Berkeley, Berkeley, CA; [3]US Department of Agriculture-Agricultural Research Service, Albany, CA; [4]Kearney Agricultural Research & Extension Center, Parlier, CA; [5]Westside Research & Extension Center, University of California, Davis, Five Points, CA*

MP 625 **Utilization of Substructure Identification through MSn Analysis for Unknown Structure Determination Assisted with in silico Fragmentation Prediction**; Tim Stratton; *Thermo Fisher Scientific, San Jose, CA*

MP 626 **Spatial Distribution Mapping of Molecules in the Grains of Different Rice Landraces, Using Desorption Electrospray Ionization Mass Spectrometry**; Arunan Suganya[1]; Debal Deb[2]; Thalappil Pradeep[1]; *[1]Indian Institute of Technology - Madras, Chennai, India; [2]Centre for Interdisciplinary Studies, Barrackpore, Kolkata 700 123, India*

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MP 627 **Gaseous Polylactide Ions Retain Structural Memory of How They Were Produced by ESI: An Ion Mobility Spectrometry/Molecular Dynamics Simulation Study**; Quentin Duez[1,2]; Haidy Metwally[2]; Sébastien Hoyas[1]; Vincent Lemaur[1]; Jérôme Cornil[1]; Pascal Gerbaux[1]; Lars Konermann[2]; Julien De Winter[1]; *[1]University of Mons, Mons, Belgium; [2]University of Western Ontario, London , ON*

MP 628 **Analysis of an Ethoxylated Capyrlic/Capric Polyglyceride Surfactant Mixture *via* Liquid Chromatography Coupled to Ion Mobility Mass Spectrometry**; Jason Michael O'neill[1]; Chrys Wesdemiotis[1]; *[1]The University of Akron Chemistry Department, Akron, OH*

MP 629 **A Mass Spectrometry Imaging Method for Visualizing Synthetic Polymers Combining with Kendrick Mass Defect Analysis**; Takaya Satoh[1]; Sayaka Nakamura[2]; Thierry Fouquet[2]; Hiroaki Sato[2]; Yoshihisa Ueda[3]; Mike H. Frey[4]; *[1]JEOL Ltd. MSBU Application division Group1, Akishima, Tokyo, Japan; [2]Research Institute for Sustainable Chemistry, National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan; [3]JEOL Ltd. MSBU,, Akishima, Japan; [4]JEOL USA, Inc., Peabody, MA*

MP 630 **Molecular Coding/Decoding of Oligomer Sequences via Advanced Polymer Chromatography – Ion Mobility Separation - Mass Spectrometry Hyphenation**; Marie-Theres Picker[1]; Chiel Mertens[2]; Filip Du Prez[2]; Dirk Kuckling[1]; *[1]Paderborn University, Paderborn, Germany; [2]Ghent University, Ghent, Belgium*

MP 631 **Characterization of MQ Silicone Resins by GPC-MALDI-MS**; Tianlan Zhang[1]; Wei Gao[1]; Donald Eldred[2]; Tom Bekemeier[2]; *[1]The Dow Chemical Co, Collegeville, PA; [2]Dow Chemical Company, Auburn, MI*

MP 632 **Molecular Characterization of Oligomeric Pyrolysis Compounds of Ethyl Acrylate-Butyl Acrylate Copolymer Using Thermal Desorption/Pyrolysis DART-MS**; Chikako Takei[1]; Kenichi Yoshizawa[1]; Sayaka Nakamura[2]; Hiroaki Sato[2]; Hajime Ohtani[3]; *[1]BioChromato, Inc., Fujisawa, Japan; [2]National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan; [3]Nagoya Institute of Technology, Nagoya, Japan*

MP 633 **Structural Elucidation of Multiply Charged Gaseous Organosilicon Cations *via* Solution Phase Additives**; Tanya Habitz[1]; Ron Tecklenburg[1]; John Stutzman[1]; *[1]The Dow Chemical Company, Midland, MI*

MP 634 **Optimizing the Performance of Organic Memory Devices – A Complementary Multi-Technique Analytical Approach**; Lothar Veith[1]; Minye Jin[1]; Hans Joachim Räder[1]; Jasper Michels[1]; Rüdiger Berger[1]; Paul Blom[1]; Tanja Weil[1]; *[1]Max Planck Institute for Polymer Research, Mainz, Germany*

MP 635 **A Study on Matrix Preparation towards MALDI-Imaging of Synthetic Polymer Samples**; Toshiji Kudo[1]; Takashi Nirasawa[2]; Shigeru Sakamoto[1]; *[1]Bruker Japan K.K., Yokohama, Japan; [2]Bruker Japan K.K., Yokohama, Japan*

MP 636 **A High Performance Liquid Chromatography/Mass Spectrometry (LC/MS) Method for the Characterization of Stressed Polysorbate 20 and 80**; Paul W. Brown[1]; Yan He[1]; Olga Friese[2]; Jason Rouse[3]; *[1]Pfizer, Wildwood, MO; [2]Pfizr, Wildwood, MO; [3]Pfizer, Andover, MA*

MP 637 **Chemical Depolymerization and Analysis of Synthetic and Natural Insoluble Polymers by 1D and 2D High Resolution FT-ICR Mass Spectrometry**; Ziad Mahmoud[1]; Sergui Mansour[1]; Fabrice Bray[1]; Laëtitia Chausset-Boissarie[1]; Christian Rolando[2]; *[1]Université de Lille, Villeneuve d'Ascq, France; [2]Univ. de Lille, Sciences et Technologies, Villeneuve D'ascq, France*

MP 638 **Determination of the Detailed Electron Impact Fragmentation Pathways for Mercaptopropyl and Chloropropyl Containing Silane Coupling Agents and Siloxane Polymers**; Ron Tecklenburg[1]; Tanya Habitz[1]; *[1]The Dow Chemical Company, Midland, MI*

MP 639 **ケンド(リック): "Kendo" Open File for the Advanced Kendrick Mass Defect Analysis of Mass Spectra From Polymeric Materials**; Thierry Nicolas Jean Fouquet[1]; Sayaka Nakamura[1]; Robert Cody[2]; Hiroaki Sato[1]; *[1]National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan; [2]JEOL USA, Inc., Peabody, MA*

PROTEIN THERAPEUTICS: QUANTITATIVE ANALYSIS I
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MP 640 **Effect of Amino Acid Supplementation on Host Cell Protein Profile for Recombinant *Pramlintide concatemer* Production in *E. coli***; Rohan Shah[1]; Saurabh Nagpal[2]; Anurag Rathore[1]; Jashwant Kumar[1]; *[1]Indian Institute of Technology, delhi, India; [2]Agilent Technologies, Gurgaon, India*

MP 641 **Compiling a Method Toolbox to Improve Detection of Host Cell Proteins**; Martha Stapels[1]; Helena Awad[1]; Michelle Busch[1]; Joanne Cotton[1]; Fateme Tousi[1]; *[1]Sanofi, Framingham, MA*

MP 642 **Monitoring of Non-Human Glycan Motif in Biotherapeutics for Immunogenicity Prediction**; Unyong Kim[1]; Myung Jin Oh[2,3]; Nari Seo[2,3]; Hyun Joo An[2,3]; *[1]GLYCAN Co., Ltd., Seongnam, South Korea; [2]Asia-Pacific Glycomics Reference Site, Daejeon, South Korea; [3]Chungnam National University, Daejeon, South Korea*

MP 643 **Quantitative Analysis of Intact Monoclonal Antibodies from Mouse Serum Using LC/MS and CE/MS Techniques**; David Wong[1]; Omar S. Bamaby[2]; Mei Han[3]; Yanan Yang[3]; Christopher A. James[4]; *[1]Agilent Technologies, Inc., Santa Clara, CA; [2]Amgen, Inc., Thousand Oaks, CA; [3]Amgen Inc., South San Francisco, CA; [4]Amgen, Inc., Thousand Oaks, CA*

MP 644 **Spatially-Resolved, 3D-Printed Micro-Sampling Coupled to Sensitive Nano-LC-MS to Quantify the Absolute Levels of Heterogeneous Distribution of mAb/Targets in Tissues**; Ming Zhang[1]; Bo An[1]; Jun Qu[1]; *[1]SUNY at Buffalo, Buffalo, NY*

MP 645 **Characterization of Commercial Vaccines by Charge Detection Mass Spectrometry**; Kevin Bond[1]; Che-Yen (Joe) Wang[2]; Martin F Jarrold[1]; *[1]Indiana University Bloomington, Bloomington, IN; [2]Indiana University, Bloomington, IN*

MP 646 **High-Resolution Isolation LC/SRM-MS Enabled Improved Selectivity *via* the Isolated Isotopic Precursor/Product Transitions**; Shihan Huo[1]; Jie Pu[1]; Ming Zhang[1,2]; Xiaoyu Zhu[1]; Jun Qu[1,2]; *[1]University at Buffalo, Buffalo, NY; [2]New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, NY*

MP 647 **A Peptide Mapping Based Quality-by-Design Study of Biopharmaceuticals Oxidation during Formulation Development**; Bo Zhai[1]; Danika Rodrigues[2]; Dwaine Banton[3]; Andrew D Mahan[1]; Stuart Ember[2]; Jeffrey Brelsford[1]; Santosh Thakkar[2]; Hirsh Nanda[1]; *[1]Janssen Research & Development, Cell & Developability Sciences, Spring House, PA; [2]Janssen Research & Development, Large Molecule Drug Product Development, Malvern, PA; [3]Janssen Research & Development, Manufacturing and Applied Statistics, Spring House, PA*

MP 648 **A Generic Anti-Peptide Capture Coupled to LC/MS MRM for Low Level Pharmacokinetic Measurements of Therapeutic Proteins**; Bao-Jen Shyong[1]; Weixun Wang[2]; Huaibing He[2]; Bernard Choi[2]; Lucinda Hittle[2]; Kevin Bateman[1]; Daniel Spellman[1]; *[1]Merck & Co., Inc., West Point, PA; [2]Merck & Co., Inc., Rahway, NJ*

MP 649 **Comparison of Methods for Plate-Based Capture and Quantification of Monoclonal Antibodies by LC-MS**; Nicolas Caffarelli[1]; Yue Lu[1]; Pegah Jalili[1]; Thomas Juehne[1]; Jeffrey Turner[1]; Kevin Ray[1]; *[1]MilliporeSigma, St. Louis, MO*

MP 650 **Engineering the XS® Pichia Expression System to Reduce Host Cell Protein Impurities in Biopharmaceuticals Production**; Sylwia Jozwiak[1]; Katrien Claes[2]; Christoph Kiziak[2]; James Graham[1]; *[1]Research and Development, Pharma&Biotech, Lonza Biologics plc, Slough, United Kingdom; [2]Research and Development Microbial, Pharma&Biotech, Lonza AG, Visp, Switzerland*

MP 651 **A High-Resolution Multi-Attribute Method for Product Characterization, Process Characterization, and Quality Control of Therapeutic Proteins**; Xiaoyan Guan[1]; Le Zhang[1]; Da Ren[1]; Tamer Eris[1]; *[1]Amgen, Thousand Oaks, CA*

MP 652 **The Development of a Point-of-Need Miniaturized ESI-MS for Upstream Bioprocessing Applications**; Richard W Moseley[1]; Alex I McIntosh[1]; *[1]Microsaic Systems, Woking, United Kingdom*

MP 653 **Evaluation of nSMOL Methodology for the Analysis of the mAb Bevacizumab in Human Plasma by LC-MS/MS**; Mike Buonarati[1]; Stephen Kurzyniec[2]; Vikki Johnson[2]; Reed Lyon[1]; Laurence M. Brill[1]; Dale Schoener[1]; *[1]Intertek Pharmaceutical Services, San Diego, CA; [2]Shimadzu Scientific Instruments, Inc, Carlsbad, CA*

MP 654 **Comprehensive and Streamlined Approach for Host Cell Protein Identification and Quantification**; Sean McCarthy[1]; Zoe Zhang[2]; Lei Xiong[2]; Elliott Jones[2]; *[1]SCIEX, Framingham, MA; [2]Sciex, Redwood City, CA*

MP 655 **Tandem Quadrupole MS for the Quantification of Monoclonal Antibody Subunit Light Chains in Plasma**; Caitlin M Dunning[1]; Mary E Lame[1]; Yun W Alelyunas[1]; Mark D Wrona[1]; *[1]Waters Corporation, Milford, MA*

MP 656 **Comparison of Sample Preparation Methods for Hybrid Ligand Binding Assay-Liquid Chromatography Tandem Mass Spectrometry**; Maria-Christina S Malinao[1]; Chad Eichman[1]; Brian Rivera[1]; *[1]Phenomenex, Torrance, CA*

MP 657 **An Improved Immunoaffinity LC-MS/MS Workflow for the Quantitation of IgG's during Preclinical PK Studies**; Michael M. Rosenblatt[1]; Iyndsey Jager[1]; Nidhi Nath[1]; Marjeta Urh[1]; *[1]Promega Corporation, Madison, WI*

MP 658 **Ultra-sensitive Quantification of Monoclonal antibodies and ADCs in Mouse Plasma using Trap-Elute MicroLC-MS/MS method**; Lei Xiong[1]; Ji Jiang[1]; Remco van Soest[1]; *[1]Sciex, Redwood City, CA*

MP 659 **Efficient Data Processing Workflows for In-Depth, MS-Based Glycoanalysis of Biopharmaceuticals**; Aude Tartiere[1]; Albert Van Wyk[2]; Joe Shambaugh[3]; John McCarter[3]; Cassandra Wigmore[4]; Peter Haberl[5]; *[1]Genedata, Inc., San Francisco, CA; [2]Genedata Ltd, Cambridge, United Kingdom; [3]Genedata Inc, Lexington, MA, USA, Lexington, MA; [4]Genedata AG, Basel, Switzerland, Basel, Switzerland; [5]Genedata GmbH, Munich, Germany, Munich, Germany*

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MP 660 **Isotopically Resolved Analysis of Protein Subunits Using High Resolution Accurate Mass**; Sean McCarthy[1]; Melanie Juba[2]; Zoe Zhang[3]; *[1]SCIEX, Framingham, MA; [2]Sciex, Framingham, MA; [3]Sciex, Redwood City, CA*

MP 661 **Laser-Free FPOP Hydroxyl Radical Protein Foot-Printing with In-Line Radical Dosimetry for Biopharmaceutical Higher Order Structural Analys**; Scot R Weinberger[1]; Ron C. Orlando[1, 2]; Joshua S Sharp[1, 3]; *[1]GenNext Technologies, Inc., Montara, CA; [2]University of Georgia, Athens, GA; [3]University of Mississippi, University, MS*

MP 662 **Mass Spectrometric Characterization of Acidic Species Generated in Cell Culture and Stability Studies of Monoclonal Antibodies**; Ioannis A Papayannopoulos[1]; Shannon Renn-Bingham[1]; *[1]Celldex Therapeutics, Fall River, MA*

MP 663 **Mapping Glycation Sites of an Antitumor Tn-BSA Neoglycoconjugate by Mass Spectrometry**; Simin Tavangari[1]; Rene Roy[1]; Alexandra M Furtos[2]; *[1]Universite du Quebec a Montreal, Montreal, Québec; [2]University of Montreal, Montreal, QC*

MP 664 **A Single Injection LC-MS Analysis Scheme for Simultaneous Analysis of Biotherapeutics and Host-Cell Impurities *via* Online Digestion LC-MS/MS**; Joshua Emory[1]; Brian Feild[1]; Harsha P. Gunawardena[2]; *[1]Shimadzu Scientific Instruments, Inc., Columbia, Maryland; [2]Janssen Research and Development, Spring House, PA*

MP 665 **On-Line Aggregate and Fragment Analysis of Therapeutic Monoclonal Antibodies Using Native Size Exclusion Chromatography Mass Spectrometry**; Chongfeng Xu[1]; Zoran Sosic[1]; Sean McCarthy[2]; Esme Candish[2]; Fan Zhang[3]; Elliott Jones[2]; *[1]Biogen, Cambridge, MA; [2]Sciex, Framingham, MA; [3]Sciex, Redwood City, CA*

MP 666 **Hydroxyl Radical Protein Footprinting Reveals Buffer Effects in Adalimumab Biosimilar Aggregation and Heat Shock Tolerance**; Joshua S. Sharp[1]; Sandeep K. Misra[1]; Scot R Weinberger[2]; Ron C. Orlando[2, 3]; *[1]University of Mississippi, University, MS; [2]GenNext Technologies, Inc., Montara, CA; [3]University of Georgia, Athens, GA*

MP 667 **CESI-MS: A Useful Tool to Analyze the Charge Variants and Disulfide Structural Heterogeneity of IgG2**; Prashant Dour[1]; Faraz Rashid[1]; Dipankar Malakar[1]; Manoj Pillai[1]; *[1]SCIEX INDIA, Gurugram, India*

MP 668 **Structural Study of a PEGylated Therapeutic Protein by MALDI-ISD and ESI-QTOF**; Sergei Dikler[1]; Anjali Alving[1]; *[1]Bruker Scientific, Billerica, MA*

MP 669 **Automated Chemical Footprinting Enables Monitoring of Conformational Change of Protein Therapeutics**; Sonya Entova[1]; Nina Chen[1]; Mohammed Sahar[1]; Alla Polozova[1]; Hao Zhang[1]; *[1]Amgen Inc., Cambridge, MA*

MP 670 **Time-resolved Deconvolution for Automated, In-depth Characterization of an IgG-type Monoclonal Antibody by Intact Mass Analysis**; Peter Haberl[1]; John McCarter[2]; Aude Tartiere[3]; Albert Van Wyk[4]; Cassandra Wigmore[5]; Joe Shambaugh[2]; *[1]Genedata GmbH, Munich, Germany; [2]Genedata, Inc., Lexington, MA; [3]Genedata, Inc., San Francisco, CA; [4]Genedata Ltd, Cambridge, United Kingdom; [5]Genedata AG, Basel, Switzerland*

MP 671 **Improving Sequence Coverage of Hydrophobic Regions of Bispecific Antibody Cancer Therapeutics with Top-Down Mass Spectrometry and Enzymatic Digestion**; Jennifer Lippens[1]; Burton Lee[1]; Andrew Dykstra[1]; Tawnya Flick[1]; *[1]Amgen, Inc., Thousand Oaks, CA*

MP 672 **A Workflow-Driven Platform Solution for MAM-Based Critical Quality Attribute Monitoring of Biotherapeutics in Process Development and QC**; Nilini Ranbaduge[1]; Henry Shion[1]; Ying Qing Yu[1]; Min Du[1]; Weibin Chen[1]; *[1]Waters Corporation, Milford, MA*

MP 673 **Characterization and Relative Quantitation of Sequence Variants in Protein Therapeutics by Liquid Chromatography Tandem Mass Spectrometry**; Scott Ugrin[1]; Colin G. Barry[1]; Michelle English[2]; *[1]Alliance Pharma, Malvern, PA; [2]Protein Metrics Inc., San Carlos, CA*

MP 674 **High-Throughput Analysis of Antibody Charge Heterogeneity by Native Microfluidic Capillary Electrophoresis- Mass Spectrometry**; Hongxia (jessica) Wang[1]; Haibo Qiu[1]; Jikang Wu[1]; Thomas Daly[1]; Ning Li[1]; *[1]Regeneron Pharmaceuticals Inc., Tarrytown, NY*

MP 675 **Streamlining mAb Characterization with a PASEF Based Disulfide Analysis Workflow**; Stuart Pengelley[1]; Waltraud Evers[1]; K. Ilker Sen[2]; Guillaume Tremintin[3]; Eric Carlson[2]; Detlev Suckau[1]; Anja Resemann[1]; Marshall Bern[2]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Protein Metrics Inc., Cupertino, CA; [3]Bruker Daltonics Inc., Billerica, MA 01821*

MP 676 **Improved Middle-Down Characterization of Antibodies Using Multiple Ion Activation Techniques and Proton Transfer Reaction on a Modified Orbitrap Mass Spectrometer**; Romain Huguet[1]; Kristina Srzentic[2]; John E. P. Syka[1]; Christopher Mullen[1]; Joshua A Silveira[1]; Jennifer Sutton[1]; Luca Fornelli[3]; *[1]Thermo Fisher Scientific, San Jose,*

CA; [2]Thermo Fisher Scientific, Cambridge, MA; [3]University of Oklahoma, Health and Science Center, Norman, OK

MP 677 **Optimization of Capillary Nondenaturing Size Exclusion Chromatography of Proteins Coupled to a Multinozzle Electrospray Source**; Theresa McLaughlin[1]; Yue Ju[2]; Pan Mao[3]; Guillaume Tremintin[4]; Allis S. Chien[1]; Mei Park[4]; *[1]Stanford University, Stanford, CA; [2]Bruker Daltonics Inc., Billerica, MA 01821; [3]Newomics Inc., Berkeley, CA; [4]Bruker Daltonics Inc., Billerica, MA*

MP 678 **Data Independent Top-down Mass Spectrometry Facilitated by a New MSE Processing Tool**; Lindsay J Morrison[1]; Barbara J Sulivan[1]; *[1]Waters Corporation, Beverly, MA*

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MP 679 **Composition and Particle Size Characterization of ApoL1 Containing Molecular Assemblies in Human Plasma in Relation to Kidney Filtration Rate**; Michael Andrews[1]; Andrew N Hoofnagle[2]; Yulanda Williamson[1]; David Schieltz[1]; Zsuzsanna Kuklenyik[1]; John R Barr[1]; *[1]Centers for Disease Control and Prevention, Chamblee, GA; [2]University of Washington, Seattle, WA*

MP 680 **The Investigation of High Intensity Interval Training on Left Ventricular Fibrosis in Cardiac Patients by Proteomics**; Meng-chu Liu[1]; Pang-Hung Hsu[1]; Chih-Chin Hsu[2]; *[1]Department of Bioscience and Biotechnology, National Taiwan Ocean University, Keelung City, Taiwan; [2]Department of Physical Medicine and Rehabilitation, Keelung Chang Gung Memorial Hospital, Keelung City, Taiwan*

MP 681 **Total Solubilization of FFPE Samples for One Pot High Throughput, High Yield Clinical Proteomics**; John P. Wilson[1]; Ilyana Ilieva[2]; Darryl J Pappin[1, 3]; John B. Wojcik[2]; *[1]ProtiFi, LLC, Farmingdale, NY; [2]University of Pennsylvania, Philadelphia, PA; [3]Cold Spring Harbor laboratory, Cold Spring Harbor, NY*

MP 682 **Identification of Aggressive Prostate Cancers: In-depth Proteomics of Tissues and Urines**; Andrew Maclin[1]; Amanda Khoo[2]; Katharina Fritsch[2]; Ankit Sinha[2]; Vladimir Ignatchenko[1]; Joseph J. Otto[3]; Lydia Y. Liu[2]; Vincent Huang[4]; Julie Livingstone[4]; Danny Vesprini[5]; Julius O. Nyalwidhe[3]; O. John Semmes[3]; Paul C. Boutros[6]; Stanley Liu[5]; Thomas Kislinger[1]; *[1]Princess Margaret Cancer Centre, Toronto, ON; [2]University of Toronto, Toronto, ON; [3]Eastern Virginia Medical School, Norfolk, VA; [4]Ontario Institute for Cancer Research, Toronto, ON; [5]Sunnybrook Health Sciences Centre, Toronto, ON; [6]UCLA, Los Angeles, CA*

MP 683 **Identifying Quantitative Protein Changes in the Iris of Glaucoma Patients Using Label Free Proteomics**; Craig P Dufresne[1]; Richard D Semba[2]; Pingbo Zhang[2]; Min Zhu[2]; Jiang Qian[3]; Tianshun Gao[2]; Ibrahim AlJadaan[4]; Sami AlShahwan[4]; Ohood Owaidha[4]; Randy Craven[2]; Deepak Edward[2, 4]; Alka Mahale[4]; *[1]Thermo Fisher Scientific, West Palm Beach, FL; [2]Johns Hopkins University, Baltimore, MD; [3]National Institute on Aging, National Institutes of Health, Baltimore, MD; [4]King Khaled Eye Specialist Hospital, Riyadh, Saudi Arabia*

MP 684 **Protein Signatures for Diagnosis of Ovarian Cancer in a Murine Model**; Melissa M Galey[1]; Alexandria N Young[1]; Valentina Petukhova[1]; Jian Wang[2]; Mingxun Wang[2]; Joanna E Burdette[1]; Laura M Sanchez[1]; *[1]University of Illinois at Chicago, Chicago, IL; [2]Ometa Labs, San Diego, CA*

MP 685 **Application of Plasma Proteomics in Alzheimer's Disease**; Mostafa J Khan[1]; Renã A.S. Robinson[1]; *[1]Vanderbilt University, Nashville, TN*

MP 686 **Using iTRAQ-labeling nanoLC-MS/MS Proteomic Approaches to Discovery Urinary Protein Biomarkers of Urothelial Carcinoma**; Chao-Jung Chen[1]; Chieh Yang[2]; Che-Yi Chou[1, 3]; Chiu-Ching Huang[4, 5]; *[1]China Medical University, Taichung, Taiwan; [2]China Medical University Hospital, Taichung, Taiwan; [3]Asia University Hospital, Taichung, Taiwan; [4]China Medical University Hospital, Taichung, Taiwan; [5]China Medical University, Taichung City, Taiwan*

MP 687 **Proteomics Analysis of Acid Bone Lysate Using Micro Pillar Arrayed Columns**; Goran Mitulovic[1]; Franz Josef Strauss[2, 3]; Alexandra Stähli[2, 4]; Lucian Beer[2]; Valentina Gilmozzi[2]; Nina Haspel[2]; Gerhild Schwab[2]; Rainhard Gruber[2]; *[1]Medical University of Vienna, KIMCL, Vienna, Austria; [2]Medical University of Vienna, Vienna, Austria; [3]University of Chile, Santiago, Chile; [4]University of Bern, Bern, Switzerland*

MP 688 **Optimized Sample Preparation for the Assessment of Formalin-Fixed and Paraffin Embedded (FFPE) Tissue Specimen for Mass-Spectrometry Based Proteogenomics**; Georgia Mitsa[1]; Adriana Aguilar[2]; Mark Basik[3]; Sonia del Rincon[1]; Rene Zahedi[1]; Christoph H. Borchers[1, 3, 4, 5]; *[1]Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; [2]Segal Cancer Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; [3]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC; [4]University of Victoria-Genome BC Proteomics Centre, Victoria, BC; [5]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC*

MP 689 **Proteomic Analysis of Dpy19l2-Deficient Human Globozoospermia Reveals Multiple Molecular Defects**; Xuejiang Guo[1]; Yueshuai Guo[1]; Daozhen Chen[2]; Xiaoyu Yang[1]; *[1]Nanjing Medical University, Nanjing, China; [2]Wuxi Maternal and Child Health Care Hospital Affiliated to Nanjing Medical University, Wuxi, China*

MP 690 **Mass Spectrometry-Based Proteomes of Paired Human Cerebrospinal Fluid and Plasma in Relation to the Blood-Brain Barrier**; Loïc Dayon[1]; Ornella Cominetti[1]; Jérôme Wojcik[2]; Antonio Núñez Galindo[1]; Aikaterini Oikonomidi[3]; Hugues Henry[4]; Eugenia Migliavacca[1]; Martin Kussmann[1, 5]; Gene L. Bowman[1, 6, 7]; Julius Popp[3, 8]; *[1]Nestlé Institute of Health Sciences, Nestlé Research, Lausanne, Switzerland; [2]Precision for Medicine, Geneva, Switzerland; [3]CHUV, Old Age Psychiatry, Department of Psychiatry, Lausanne, Switzerland; [4]CHUV, Department of Laboratories, Lausanne, Switzerland; [5]Frontiers Media S.A., Lausanne, Switzerland; [6]Marcus Institute for Aging Research, Hebrew Senior Life, Boston, MA; [7]Department of Medicine, Beth Israel Deaconess Medical Center and Harvard Medical School, Boston, MA; [8]HUG, Geriatric Psychiatry, Department of Mental Health and Psychiatry, Geneva, Switzerland*

MP 691 **Proteomic Characterisation of Chronic Lymphocytic Leukaemia Identifies Putative Subtype-Independent Clinical Targets and Dysregulation of the Spliceosome**; Harvey Johnston[1, 2]; Matthew J Carter[2]; Marta Larrayoz[2]; James Clarke[2]; Spiros D Garbis[2]; David Oscier[2]; Jonathan C Strefford[2]; Andrew J Steele[2]; Renata Walewska[2]; Mark S Cragg[2]; *[1]UCL, London, United Kingdom; [2]University of Southampton, Southampton, United Kingdom*

MP 692 **Proteomic Characterization of Microneedle-Extracted Dermal Interstitial Fluid**; Gabrielle Rizzo[1]; Bao Q. Tran[2]; Phillip Miller[3]; C Nicole Rosenzweig[4]; Ronen Polsky[3]; Trevor Glaros[4]; Phillip Mach[5]; *[1]Excet, Inc., Springfield, VA; [2]20th CBRNE Command, APG, MD; [3]Sandia National Laboratory, Albuquerque, NM; [4]ECBC, Aberdeen Proving Ground, MD; [5]US Army ECBC, Aberdeen Proving Ground, MD*

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MP 693 **MiCIdGUI: A User Friendly Graphical Interface for MiCId a Tool for Microorganism Classification and Identification**; Gelio Alves[1]; Aleksey Ogurtsov[1]; Oleg Obolensky[1]; Yi-Kuo Yu[1]; *[1]National Center for Biotechnology Information, NLM, Bethesda, MD*

MP 694 **MHCquant: Automated and Reproducible Data Analysis for Immunopeptidomics**; Leon Bichmann[1]; Annika Nelde[2, 3]; Michael Ghosh[2]; Timo Sachsenberg[1]; Christopher Mohr[4]; Alexander Peltzer[4]; Leon Kuchenbecker[1]; Juliane S. Walz[3]; Stefan Stevanović[2, 5]; Hans-Georg Rammensee[2, 5]; Oliver Kohlbacher[1, 4, 6, 7]; *[1]Applied Bioinformatics, Department of Computer Science, University of Tübingen, Tübingen, Germany; [2]Institute for Cell Biology, Department of Immunology, University of Tübingen, Tübingen, Germany; [3]Department of Hematology and Oncology, University of Tübingen, Tübingen, Germany; [4]Quantitative Biology Center, University of Tübingen, Tübingen, Germany; [5]German Cancer Consortium (DKTK), DKFZ partner site, Tübingen, Germany; [6]Biomolecular Interactions, Max Planck Institute for Developmental Biology, Tübingen, Germany; [7]Institute for Translational Bioinformatics, University Hospital Tübingen, Tübingen, Germany*

MP 695 **Evaluation of Instrumental Variability Utilizing 2D LC-MS/MS Proteomic HeLa Standard Data to Enhance Quality Control Metrics in Clinical Proteomics**; Richard M. Searfoss[1]; Punit Shah[1]; Kennedy Ofori-Mensa[1]; Kiki Panagopoulos[1]; Rangaprasad Sarangarajan[1]; Niven R. Narain[1]; Michael A. Kiebish[1]; *[1]BERG, LLC, Framingham, MA*

MP 696 **Plasma-Based Protein Panel Can Predict Risk of Acute Graft-Versus-Host Disease and Non-Relapse Mortality in Patients Undergoing Allogeneic Hematopoietic Stemcell Transplantation**; Kisoon Dan[1]; Junghoon Shin[2]; Dohyun Han[1]; Ji-Won Kim[3]; Kyungkon Kim[4]; Sang Hoon Song[2]; Inho Kim[2]; *[1]Proteomics Core Facility, Biomedical Research Institute, Seoul National University Hospital, Seoul, South Korea; [2]Department of Internal Medicine, Seoul National University Hospital, Seoul, South Korea; [3]Department of Internal Medicine, Seoul National University Bundang Hospital, Seongnam, South Korea; [4]Department of Convergence Medicine, Asan Institute for Life Sciences, Asan Medical Center, Seoul, South Korea*

MP 697 **Proteomic Analysis of Liver Tissue Reveals Chronic Low Level Oxidative Stress in a Mouse Model of Primary Hyperoxaluria Type 1**; Brianna E Buchalski[1]; John Knight[1]; Ross Holmes[2]; James A Mobley[3]; *[1]University of Alabama at Birmingham, Birmingham, Alabama; [2]University of Alabama at Birmingham, AL; [3]University of Alabama at Birmingham, AL*

MP 698 **Profiling of Advanced Glycation End Products (AGE) PTM on Antigen Processing Machinery and MHC-II Molecules in Diabetes and T2DM Syndrome**; Cristina C Clement[1]; Pia Negroni[2]; Kateryna Morozova[1]; Lawrence Stern[2]; Laura Santambrogio[1]; *[1]Albert Einstein College of Medicine, Bronx, NY; [2]University of Massachusetts Medical School, Worcester, MA*

MP 699 **Parallelizable Quantitative Characterization of Proteome and Targeted Metabolome from Laser Capture Microdissected Tissue Cells**; Shichen Shen[1]; Jun Li[1]; Min Ma[2]; Sailee Rasam[1]; Xiaotao Duan[3]; Jun Qu[1]; *[1]University at Buffalo, Buffalo, NY; [2]Roswell Park Comprehensive Cancer Center, Buffalo, NY; [3]Beijing Institute of Pharmacology and Toxicology, Beijing, China*

MP 700 **Kinome Profiling Identifies Drug Resistance Pathways in Hepatocellular Carcinoma**; Martin Golkowski[1]; Ho-Tak Lau[1]; Marina Chan[2]; Heidi Kenerson[3]; Venkata Narayana Vidadala[4]; Anna Shoemaker[1]; Dustin J Maly[4]; Raymond S Yeung[3]; Taranjit S Gujral[2]; Shao-En Ong[1]; *[1]Department of Pharmacology, University of Washington, Seattle, WA; [2]Human Biology Division, Fred Hutchinson Cancer Research Center, Seattle, WA; [3]Department of Surgery, University of Washington, Seattle, WA; [4]Department of Chemistry, University of Washington, Seattle, WA*

MP 701 **Contraceptive Pills Alter Proteome of Erythrocytes and Induce Redox Damages**; Laurence Servais[1]; Clovis Wouters[1]; France Baumans[1]; Dominique Baiwir[2]; Irina Lobysheva[3]; Flavia Dei Zotti[3]; Edwin De Pauw[1]; Gauthier Eppe[1]; Jean-Luc Balligand[3]; Gabriel Mazzucchelli[1, 2]; *[1]University of Liege, Mass Spectrometry Laboratory, MolSys Research Unit, Liege, Belgium; [2]University of Liège, GIGA Proteomics Facility, Liege, Belgium; [3]Institute for Experimental and Clinical Research (IREC) and Pole of Pharmacology and Therapeutics (FATH)/UCL, Brussels, Belgium*

MP 702 **A Fast Sample Processing Strategy for Deep Urine Label-Free Quantification Proteomic Analysis**; Pamela S Cantrell[1]; Xuemei Zeng[1]; Nathan A Yates[1, 2]; *[1]Biomedical Mass Spectrometry Center, University of Pittsburgh Schools of the Health Sciences, Pittsburgh, PA; [2]Department of Cell Biology, University of Pittsburgh School of Medicine, Pittsburgh, PA*

MP 703 **Method Development for the Identification of Proteins in Fingertip Smears by Using MALDI-MS**; Cristina Russo[1]; Laura Cole[1]; Lynda Wyld[2]; Simona Francese[1]; *[1]Sheffield Hallam University, Sheffield, United Kingdom; [2]The University of Sheffield, Sheffield, United Kingdom*

MP 704 **Carbonylated Proteome Signatures Caused by Stress during Development of Human Pregnancy in GARBH-Ini cohort**; Abhishek Kumar Singh[1]; Amit Kumar Dey[1]; Pallavi Kshetrapal Kshetrapal[2]; Nitya Wadhwa[2]; Shinjini Bhatnagar[2]; Arindam Maitra[3]; Dipankar Malakar[4]; Faraz Rashid[4]; Manoj Pillai[4]; Dinakar M Salunke[5]; Tushar Kanti Maiti[1]; *[1]Regional Centre for Biotechnology, Faridabad, India; [2]Translational Health Science and Technology Institute, Faridabad, India; [3]National Institute of Biomedical genomics, Kalyani, India; [4]SCIEX INDIA, Gurugram, India; [5]International Centre for Genetic Engineering and Biotechnology, Delhi, India*

MP 705 **Quantitative Mass Spectrometry-Based Global Proteome and Phosphoproteome Analyses of Thymic Epithelial Tumors (TET)**; Xu Zhang[1]; Fatos Kirkali[1]; Yue Qi[1]; Ting Huang[2]; Tapan Maity[1]; Khoa Dang Nguyen[1]; David S. Schrump[3]; Olga Vitek[2]; Arun Rajan[1]; Udayan Guha[1]; *[1]Thoracic and GI Malignancies Branch, Center for Cancer Research, NCI, NIH, Bethesda, MD; [2]Khoury College of Computer Sciences, Northeastern University, Boston, MA; [3]Thoracic Surgery Branch, Center for Cancer Research, NCI, NIH, Bethesda, MD*

MP 706 **Serum Multi-omics Revealed the Effect of Sport Activity**; Marcello Manfredi[1]; Elisa Robotti[1]; Elettra Barberis[1]; Maria Teresa Valenti[2]; Emilio Marengo[1]; *[1]University of Piemonte Orientale, Alessandria, Italy; [2]University of Verona, Verona, Italy*

MP 707 **Proteogenomics Identifies Common Drugabble Pathways in Undifferentiated Pleiomorphic Sarcoma**; Marcos Y Mayordomo[1, 2]; Javier A Alfaro[2]; Georges Bedran[1, 2]; Nathan a Grimes[3]; Larry Hayward[1]; Jakub Factor[1]; Rob O'Neill[4]; Borek Vojtesek[5]; Helen Creedon[1]; Satya Saxena[6]; Katy Teo[1]; Val Brunton[1]; Donald Salter[1]; Ted Hupp[1, 2]; Javier A Alfaro[1, 2]; *[1]University of Edinburgh, Edinburgh, United Kingdom; [2]University of Gdansk, Gdansk, Poland; [3]University of Edinburgh, Edinburgh, United Kingdom; [4]University of Cambridge, Cambridge, United Kingdom; [5]Masaryk Memorial Cancer Institute, Oncology, Czech Republic; [6]University of Baltimore, Baltimore, MD*

MP 708 **Identifying Breast Cancer Vulnerabilities by Mapping Interactome Dysregulations in Primary Tumor Samples**; Johannes Kreuzer[1]; Robert Morris[1]; Ridwan Ahmad[1]; Cyril H. Benes[1]; Dennis C. Sgroi[1]; Wilhelm Haas[1]; *[1]Massachusetts General Hospital and Harvard Medical School, Charlestown, MA*

MP 709 **A Fully GLP Compliant Multiplexed Protein Quantification MRM Assay Panel**; Paul-Gerhard Lassahn[1]; Claudia Escher[2]; Tobias Treiber[2]; Alexandre Kornfeld[1]; Jakob Vowinckel[2]; Gregor Schütze[1]; *[1]SYNLAB Analytics & Services Switzerland AG, Birsfelden, Switzerland; [2]Biognosys AG, Schlieren, Switzerland*

MP 710 **Evaluation of Different Sample Preparation Workflows for Reproducible, Quantitative, and In-Depth Analysis of Urine Proteomics**; Hua Ding[1]; Hossein Fazelinia[1]; Lynn A. Spruce[1]; Dana A. Weiss[1]; Stephen A. Zderic[1]; Steven H. Seeholzer[1]; *[1]Children's Hospital of Philadelphia, Philadelphia, PA*

MP 711 **Biomarker Discovery in Serum and Plasma Using Protein Profiling by MALDI-TOF Mass Spectrometry**; Eric Weaver[1]; Robert English[2]; Matthew Texter[2]; Ryan Walsh[2]; *[1]University of Texas, Arlington, Arlington, TX; [2]Shimadzu Scientific Instruments, Inc., Columbia, Maryland*

MP 712 **Providing Absolute Certainty without Absolute Quantity**; Meghan Bradley[1]; Christopher M. Shuford[1]; Patricia L. Holland[1]; Michael Levandoski[1]; Russell P. Grant[1]; *[1]LabCorp, Burlington, NC*

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MP 713 **MS-Based Deep Proteome Profiling of AD Related Mouse Model Defective in RNA Splicing**; Mingming Niu[1]; Ping-Chung Chen[2]; Yun Jiao[2]; Hong Wang[2]; Junmin Peng[2]; *[1]St Jude Children's Research Hospital, memphis, TN; [2]St Jude Children's Research Hospital, Memphis, TN*

MP 714 **Docosahexaenoic Acid Attenuates Metabolic Dysfunctions Induced by Lipopolysaccharide in BV-2 Microglial Cells**; Bo Yang[1,2]; Runting Li[1]; Brian P. Mooney[1,2]; Kevin L. Fritsche[1]; David Q. Beversdorf[1]; Grace Y. Sun[1]; C. Michael Greenlief[1,2]; *[1]University of Missouri, Columbia, MO; [2]Charles W. Gehrke Proteomics Center, Columbia, MO*

MP 715 **Comparison of Quantitative LC/MS/MS Plant Protein Assay Design and Impact on Precision of Results**; Kristi Harkins[1]; Danielle Baker[1]; Michaela Owens[1]; *[1]DowDuPont, Johnston, IA*

MP 716 **Increasing the Breadth and Depth of Multiplexed Quantitation Using Advanced Instrumentation and Methods**; Devin Schweppe[1]; Qing Yu[1]; Aaron Robitaille[2]; Graeme McAlister[2]; Derek J Bailey[2]; Jose Navarrete-Perea[1]; Joao A. Paulo[1]; Romain Huguet[2]; Steven Gygi[1]; *[1]Harvard Medical School, Boston, MA; [2]ThermoFisher, San Jose, CA*

MP 717 **Quantitative Proteomic Analysis of Cell Cycle Regulation in Golgi-Matrix Assembly and Disassembly**; Hye Kyong Kweon[1]; Shijiao Huang[1]; Yanzhuang Wang[1]; Philip C. Andrews[1]; *[1]University of Michigan, Ann Arbor, MI*

MP 718 **Systematic Investigation of Protein Dynamics to Unveil Their Degradation Pathways in Human Cells**; Ming Tong[1]; Ronghu Wu[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

MP 719 **Developing Mass Spectrometry Based Proteomic Methods to Identify and Quantify Protein Carbonylation in Plants**; Georgina H Charlton[1]; Cleidiane G Zampronio[1]; John Sinclair[2]; Peter Kilby[2]; Alex Jones[1]; *[1]University of Warwick, Coventry, United Kingdom; [2]Syngenta Jealott's Hill International Research Centre, Bracknell, United Kingdom*

MP 720 **Surpassing 10,000 Proteins Quantified in Human Tissue by Augmenting Single Shot Data-Independent Acquisition (DIA) with Hybrid Libraries**; Jan Muntel[1]; Tejas Gandhi[1]; Lynn Verbeke[1]; Oliver M. Bernhardt[1]; Roland Bruderer[1]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland*

MP 721 **Dynamic Proteome Changes during Macrophage Polarization Induced by Mouse Colon Cancer Cell-Derived Exosomes**; Yifan Tan[1]; Lei Sun[2]; Meishuang Yan[3]; Yang Li[3]; Lin Wu[2]; Yan Ren[1]; Xiaomin Lou[2]; Siqi Liu[1]; *[1]BGI-Shenzhen, Shenzhen, China; [2]Beijing Institute of Genomics, Beijing, China; [3]Beijing Protein Innovation, Beijing, China*

MP 722 **Proteome-Wide Differences in Turnover Rates Among Rodents are Correlated to Their Lifespans and Energetic Demands**; Kyle Swovick[1]; Kevin A Welle[1]; Jennifer R Hryhorenko[1]; Andrei Seluanov[1]; Vera Gorbunova[1]; Sina Ghaemmaghami[1]; *[1]University of Rochester, Rochester, NY*

MP 723 **Absolute and Multiplex Protein Quantification Using Cell-Free Protein Synthesis and Mass Spectrometry**; Keiko Masuda[1]; Keiko Kasahara[2]; Ryohei Narumi[2]; Yoshihiro Shimizu[3]; *[1]RIKEN, Suita, Japan; [2]National Institutes of Biomedical Innovation, Health and Nutrition, Ibaraki, Japan; [3]RIKEN, Suita, Osaka, Japan*

MP 724 **A Novel Microduplication of ARID1B: Clinical, Genetic and Proteomic Findings**; Kathleen C Lundberg[1]; Nicholas Szoko[2]; Daniela M. Schlatzer[1]; Marvin Natowicz[2]; *[1]Case Western Reserve University, Cleveland, OH; [2]Cleveland Clinic, Cleveland, OH*

MP 725 **Global Proteomics Analysis to Decipher Common Proteostatic Stress Rescue Pathways of the Antioxidants Tempol and MitoTEMPO**; Silas D Wood[1]; Maggie PY Lam[1]; *[1]Department of Medicine, Division of Cardiology, Consortium for Fibrosis Research and Translation, Anschutz Medical Campus, Aurora, CO*

MP 726 **Histone H3K56-acetylation is Epigenetic Barrier for Embryonic Stem Cell Differentiation into Trophoblasts**; Jennifer Nance[1]; Feixia Chu[1]; Thomas Fazzio[2]; Taylor Hickman[1]; Amanda Chasse[1]; *[1]University of New Hampshire, Durham, NH; [2]University of Massachusetts Medical School, Worcester, MA*

MP 727 **Increasing Protein Overlap between Multiple Isobaric Mass Tag Experiments with Comprehensive Precursor Ion Inclusion**; Simion Kreimer[1]; Robert N. Cole[1]; *[1]Johns Hopkins, Baltimore, MD*

MP 728 **Protein Assisted Digestion Improves Sensitivity of Immunocapture-MRM Method to Quantify Stool Biomarker of Colorectal Cancer**; Rebecca Bearden[1]; Baochuan Guo[1]; *[1]Cleveland State University, Cleveland, OH*

MP 729 **In vivo Protein Turnover Rates in Mouse and Human Tissues**; Brian L. Frey[1]; Zach Rolfs[1]; Xudong Shi[1]; Yoshitaka Kawai[1]; Bruce A. Buchholz[2]; Lloyd M. Smith[1]; Nathan V. Welham[1]; *[1]University of Wisconsin - Madison, Madison, WI; [2]Lawrence Livermore National Laboratory, Livermore, CA*

MP 730 **Characterization of the Ubiquitination Signaling on Hypoxia-Inducible Factor with Quantitative Chemical Proteomics Analysis**; Yunan Li[1]; Ang Luo[1]; Luke Erber[1]; Yue Chen[1]; *[1]University of Minnesota at Twin Cities, Minneapolis, MN*

MP 731 **Identification and Characterizations of O2- and O4-Alkylthymidine DNA-Binding Proteins**; Xiaomei He[1]; Pengcheng Wang[1]; Hong Wang[1]; *[1]University of California, Riverside, Riverside, CA*

MP 732 **Evaluation of the Accuracy of Synchronous Precursor Selection (SPS) in Public Datasets**; Conor Jenkins[1,2]; Aimee Rinas[3]; Benjamin Orsburn[1]; *[1]Think20 Labs, Columbia, MD; [2]Hood College Bioinformatics Program, Frederick, MD; [3]AIT BioSciences, Indianapolis, IN*

MP 733 **Applications of Mass Spectrometry Targeted Assays for Quantitative Analysis of Cancer Signaling Proteins**; Penny Jensen[1]; Bhavin Patel[1]; Leigh A Foster[1]; Aaron S. Gajadhar[2]; Sebastien Gallien[3]; Jonathan R Krieger[4]; Jiefei Tong[5]; Michael F. Moran[4]; Rosa Viner[2]; Andreas Huhmer[2]; Kay Opperman[1]; John C Rogers[1]; *[1]Thermo Fisher Scientific, Rockford, IL; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Precision Medicine Science Center, Cambridge, MA; [4]SPARC BioCentre, Hospital for Sick Children, Toronto, Ontario; [5]Program in Cell Biology, The Hospital for Sick Children, Toronto, Ontario*

MP 734 **A Modified Orbitrap™ Tribrid Mass Spectrometer with Real-Time Search and Advanced Spectral Processing Enhances Multiplexed Proteome Coverage and Quantification Accuracy**; Aaron M Robitaille[1]; Romain Huguet[1]; Derek J Bailey[1]; Graeme McAlister[1]; Arne Kreutzmann[2]; Daniel Mourad[2]; Daniel Lopez-Ferrer[1]; Andreas Huhmer[1]; Vlad Zabrouskov[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Bremen, Germany*

MP 735 **Improved Identification, Quantification Accuracy, and Workflow Efficiency Using a Modified Quadrupole Orbitrap™ Mass Spectrometer and Tandem Mass Tags™ (TMT™) Approach**; Aaron Robitaille[1]; Tabiwang N. Arrey[2]; Markus Kellmann[2]; Arne Kreutzmann[2]; Daniel Mourad[2]; Daniel Lopez-Ferrer[1]; Andreas Huhmer[1]; Alexander Harder[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Bremen, Germany*

MP 736 **Strategies for Sample Normalization Post-Acquisition for Tandem Mass Tag (TMTTM) Quantitative Workflow**; Pedro Navarro[1]; Fernando J García Marqués[2]; Woong Kim[3]; Greg Foster[3]; Sharon J. Pitteri[2]; Daniel Lopez-Ferrer[3]; *[1]Thermo Fisher Scientific, Bremen, Germany; [2]Stanford University School of Medicine, Canary Center at Stanford for Cancer Early Detection, Palo Alto, CA; [3]Thermo Fisher Scientific, San Jose, CA*

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MP 737 **Top-down Mass Spectrometry Characterization of Phospholamban Proteoforms in Cardiac Tissue Enabled by A Novel Photo-cleavable Surfactant**; Austin Carr[1]; Kyle Brown[1]; Song Jin[1]; Ying Ge[1,2,3,4]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706; [2]Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; [3]Molecular and Cellular Pharmacology Program, University of Wisconsin, Madison, WI; [4]Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI*

MP 738 **BirA* Mice Enable Cell Type Specific Proteomics *in vivo***; Shiva Ahmadi[1,2]; Elham Pourbarkhordariesfandabadi[1,2]; Angela Egert[2]; Martin Breitbach[2]; Caroline Geissen[2]; Michael Hesse[2]; Kenichi Kimura[2]; Bernd K Fleischmann[2]; Hubert Schorle[2]; Volkmar Gieselmann[1,2]; Dominic Winter[1,2]; *[1]IBMB Bonn, Bonn, Germany; [2]University of Bonn, Bonn, Germany*

MP 739 **Identification Commutability in Proteomics and Metabolomics Utilizing Human Tissue Reference Materials**; Clay Davis[1]; Benjamin Neely[1]; Tracey Schock[1]; Lisa Kilpatrick[2]; Debra Ellisor[1]; Rebecca Pugh[1]; *[1]NIST, Charleston, SC; [2]NIST, Gaithersburg, MD*

MP 740 **Alterations in Extracellular Matrix Composition during Aging and Photoaging of the Skin**; Maxwell Mccabe[1]; Kirk Hansen[1]; Ryan Hill[1]; Gary Fisher[2]; Taihao Quan[2]; *[1]University of Colorado Anschutz Medical Campus, Aurora, CO; [2]University of Michigan, Ann Arbor, MI*

MP 741 **Proteomic Profiling of Mitochondrial Complexomes; Naked Mole Rat Versus Mouse**; Satomi Miwa[1]; Andrew J Porter[1]; Graham Smith[1]; Achim Treumann[1]; Pawel Palmowski[1]; Andrei Seluanov[2]; Vera Gorbunova[2]; Thomas Von Zglinicki[1]; *[1]Newcastle University, Newcastle Upon Tyne, United Kingdom; [2]Rochester Institute of Technology, Rochester, NY*

MP 742 **Proteomics on Immune Competent Mouse Models Reveals Differences in Immunogenicity**; Fang Wang[1]; Wenyan Zhong[1]; Edward Rosfjord,[1]; Xiaoran S. Yang[1]; Luanna Lemon[1]; Jeremy S. Myers[1]; *[1]Pfizer WRD, Pearl River, NY*

MP 743 **A Proteomic Investigation of Changes in the Collagen Types Present in the Anterior Cruciate Ligament during Post-Natal Growth**; Jeffrey R. Enders[1,2]; Stephanie G. Cone[1]; Matthew B. Fisher[1]; *[1]North Carolina State University, Raleigh, NC; [2]Molecular Education, Technology, and Research Innovation Center (METRIC), North Carolina State University, Raleigh, NC*

MP 744 **Body-Wide Proteome Dynamics in the Understanding and Assessment of Multiorgan Drug Response**; Bingyun Sun; *Simon Fraser University, Burnaby, BC*

MP 745 **Bone Proteomics: Enhancing Homogenization of Bone Samples for Increased Proteomic Depth**; Rowan Matney[1]; Kratika Singhal[1]; Fang Liu[1]; Ryan D. Leib[1]; Allis S. Chien[1]; *[1]Stanford University Mass Spectrometry, Stanford, CA*

MP 746 **Elucidating Alternative Biological Pathways with Tailored Enrichment Strategies from Clinical Tissue Samples**; Kratika Singhal[1]; Rowan Matney[1]; Fang Liu[1]; Ryan Leib[1]; Allis Chien[1]; *[1]Stanford University Mass Spectrometry, Stanford, CA*

MP 747 **Distinct Blubber Proteome Responses to Single and Repeated ACTH Challenges in a Marine Mammal**; Jared Devarmin[1]; Molly McCormley[1]; Cory Champagne[2]; Alicia Stephan[1]; Laura Pujade Busqueta[1]; Dorian Houser[2]; Daniel Crocker[3]; Jane Khudyakov[1,2]; *[1]University of the Pacific, Stockton, CA; [2]National Marine Mammal Foundation, San Diego, CA; [3]Sonoma State University, Rohnert Park, CA*

MP 748 **Identification of Estradiol-Regulated Protein Networks and Associated Biological Processes in the Rat Retina by Label-Free Quantitative Proteomics**; Laszlo Prokai[1]; Khadiza Zaman[1]; Fatima Rahlouni[1]; Vien Nguyen[1]; Vladimir Shulaev[2]; Katalin Prokai-Tatrai[1]; *[1]University of North Texas Health Science Center, Fort Worth, TX; [2]University of North Texas, Denton, TX*

MP 749 **A Novel Proteomic Method Defines Extracellular Matrix Proteins and Their Post-Translational Modifications from Formalin-Fixed, Paraffin-Embedded Specimens of Heart Valve Disease**; Cassandra L Clift[1]; Susana Comte-Walters[1]; Lauren E Ball[1]; David Bichell[2]; Yan Ru Su[3]; Anand Mehta[1]; Richard R Drake[1]; Peggi M. Angel[1]; *[1]Department of Cell and Molecular Pharmacology and Experimental Therapeutics, Medical University of South Carolina, Charleston, SC; [2]Division of Pediatric Cardiac Surgery, Vanderbilt University Medical Center, Nashville, TN; [3]Department of Cardiovascular Medicine, Vanderbilt University Medical Center, Nashville, TN*

MP 750 **Comprehensive Proteomic Analysis of Gray and White Matter from Human Post-Mortem Brain Tissue**; Duc M Duong[1,2]; Luming Yin[1,2]; James J. Lah[2,3]; Allan I. Levey[2,3]; Nicholas T. Seyfried[1,2,3]; *[1]Department of Biochemistry, Emory University, Atlanta, GA; [2]Center for Neurodegenerative Diseases, Emory School of Medicine, Atlanta, GA; [3]Department of Neurology, Emory University, Atlanta, GA*

MP 751 **Proteomic Analysis of Extracellular Matrix Dynamics during Mouse Forelimb Development**; Kathryn R Jacobson[1]; Sarah L Lipp[1]; Alex R. Ocken[1]; Tamara L. Kinzer-Ursem[1]; Sarah Calve[1]; *[1]Purdue University, West Lafayette, IN*

MP 752 **Extensive Intratumor Proteogenomic Heterogeneity Revealed by Multiregion Sampling in a High-Grade Serous Ovarian Tumor Specimen**; Thomas P. Conrads[1,2]; Allison L. Hunt[1]; Guisong Wang[2]; Julie Oliver[2]; Dave Mitchell[2]; Glenn Gist[2]; Brian Hood[2]; Ming Zhou[1]; Brian Blanton[2]; Kelly Conrads[2]; Chad Hamilton[2]; Kathleen Darcy[2]; Craig Shriver[3]; Yovanni Casablanca[2]; George Larry Maxwell[2]; Nicholas W. Bateman[2]; *[1]Inova Schar Cancer Institute, Annandale, VA; [2]Gynecologic Cancer Center of Excellence, Annandale, VA; [3]John P. Murtha Cancer Center, Bethesda, MD*

MP 753 **MMP-28 Alters Immunometabolic and Bioenergetic Profile of Activated Macrophages**; Dorota Tokmina-Roszyk[1,2]; Lillian Onwuha-Ekpete[1,2]; Mohammed Refai[3]; Monika Tokmina-Lukaszewska[3]; Brian Bothner[3]; Gregg Fields[1,2]; *[1]Florida Atlantic University, Jupiter, FL; [2]The Scripps Research Institute, Jupiter, FL; [3]Montana State University, Bozeman, MT*

MP 754 **Proteomic Analysis of Human Glioblastoma Formalin-Fixed Paraffin-Embedded Tissues**; Naomi Uwugiaren[1]; Jakub Faktor[2]; David R Goodlett[1,3]; Fiona Lickiss[1,4]; Sofian Al Shboul[4]; Paul M Brennan[5]; Borek Vojtesek[2]; Theodore R Hupp[1,4]; Irena Dapic[1]; *[1]International Centre for Cancer Vaccine Science, University of Gdansk, Gdansk, Poland; [2]RECAMO, Brno, Czech Republic; [3]University of Maryland, Baltimore, MD; [4]CRUK, University of Edinburgh, Edinburgh, United Kingdom; [5]Centre for Clinical Brain Sciences, University of Edinburgh, Edinburgh, United Kingdom*

MP 755 **A Global, Multi-Regional Proteomic Map of the Human Cerebral Cortex**; Zhengguang Guo[1]; Chen Shao[2]; Yang Zhang[3]; Wenying Qiu[4]; Wenting Li[4]; Qian Yang[4]; Yin Huang[2]; Yuepan Dong[2]; Haidan Sun[5]; Xiaoping Xiao[5]; Wei Sun[5]; Chao Ma[4]; Liwei Zhang[3]; *[1]Peking Union Medicine College, Beijing, China; [2]Beijing Proteome Research Center, National Center for Protein Sciences(Beijing), Beijing Institute of Lifeomics, Beijing, China; [3]Beijing Tiantan Hospital, Capital Medical University, Beijing, China; [4]Institute of Basic Medical Sciences, Neuroscience Center, Chinese Academy of Medical Sciences, School of Basic Medicine, Peking Union Medical College, Beijing, China; [5]Institute of Basic Medical Sciences, Chinese Academy of Medical Sciences/School of Basic Medicine, Peking Union Medical College, Beijing, China*

MP 756 **Identification and Validation of Synapse-Loss Regulating Phosphorylation Events in Schizophrenia**; Megan Garver[1]; Ying Ding[2]; Robert Sweet[1]; Nathan A Yates[3]; Matthew L MacDonald[1]; *[1]UPMC, Pittsburgh, PA; [2]Department of Biostatistics, University of Pittsburgh, Pittsburgh, Pennsylvania; [3]BioMS Center, University of Pittsburgh, Pittsburgh, Pennsylvania*

MP 757 **Quantitative proteomics Analysis of Placenta from Zika Virus Infected Women**; Gabriel Borges Vélez[1]; Julio Rosado Philippi[2]; Abiel Roche Lima[1]; Kelvin Carrasquillo Carrión[1]; Yadira M Cantres Rosario[1]; Maria S Correa Rivas[3]; Loyda M Meléndez[4]; *[1]University of Puerto Rico Medical Sciences Campus, San Juan, Puerto Rico; [2]University of Puerto Rico Rio Piedras Campus, San Juan, PR; [3]University of Puerto Rico Medical Sciences Campus, Quebradillas, PR; [4]University of Puerto Rico Medical Sciences Campus, San Juan, PR*

MP 758 **Quantitative Proteogenomic Analysis of Inflamed Colon Tissue in Mice Reveals an Increase in Non-Canonical Protein Variants**; Andrew T. Rajczewski[1]; Qiyuan Han[1]; Subina Mehta[1]; Praveen Kumar[1]; Pratik D Jagtap[1]; Natalia Tretyakova[1]; Timothy J. Griffin[1]; *[1]University of Minnesota, Minneapolis, MN*

MP 759 **Interactome of the PIF Peptide (Preimplantation Factor) in Uterine Environment from Different Mammals – Proteomic Studies**; Anna Fel[1]; Paulina Czaplewska[1]; Katarzyna Macur[1]; Marcel Thiel[1]; Stanislaw Oldziej[1]; *[1]University of Gdansk, Gdansk, Poland*

MP 760 **KIT Restriction of Skin Proteome Analyzed with MALDI-Imaging Mass Spectrometry and Shotgun Proteomics on c-Kitmutant Mice**; Mayuka Kosugi[1]; Masaya Ikegawa[2,3]; Nobuto Kakuda[2]; Takashi Nirasawa[4]; Ryo Kajita[4]; Kazuo Kinoshita[5]; Yuki Kuzuhara[3]; *[1]Doshisha University, Kyotanabe City, Kyoto, Japan; [2]Graduate School, Major of Medical Life Systems, Doshisha University, Kyotanabe City, Japan; [3]Department of Medical Life Systems, Doshisha University, Kyotanabe City, Japan; [4]Bruker Japan K.K., Yokohama, Japan; [5]Shiga Medical Center Research Institute, Moriyama, Japan*

MP 761 **A Label-free Quantification Approach to Identify Differentially Expressed Proteins between Wild Type and Transgenic Alzheimer Rat Brains**; Pritha Bagchi[1]; Eric B. Dammer[1]; Geng M. Wang[1]; Robert M. Cohen[2]; Nicholas T. Seyfried[1,3]; *[1]Emory Integrated Proteomics Core, Emory University, Atlanta, GA; [2]Department of Psychiatry and Behavioral Sciences, Emory University, Atlanta, GA; [3]Department of Biochemistry, Emory University, Atlanta, GA*

MP 762 **Fast and Sensitive Quantitative Proteomic Analysis of Formalin-Fixed Paraffin-Embedded Tissue Using a Trapped Ion Mobility Q-TOF**; Matthew Willetts[1]; Shourjo Ghose[2]; Christopher Swift[2]; Gary Kruppa[2]; John P Shapiro[3]; Brad H Rovin[3]; Matthias Kretzler[4]; Jeff Hodgin[4]; *[1]Bruker, Billerica, MA; [2]Bruker Scientific, Billerica, MA; [3]The Ohio State University, Columbus, OH; [4]University of Michigan Medical School, Ann Arbor, MI*

MP 763 **Comparison of S-Trap, iST and Conventional Digestion Methods for Serum Proteomics**; Benjamin Neely[1,2]; Alison Bland[2,3]; Michael Janech[2,3]; *[1]Marine Biochemical Sciences Group, National Institute of Standards and Technology, NIST Charleston, Charleston, SC; [2]Hollings Marine Laboratory, Charleston, SC; [3]College of Charleston, Charleston, SC*

MP 764 **Quantitative Proteome and Neuropeptide Profiling in Female Pregnant Mice with Neuropathic Pain by High-Resolution Mass Spectrometry**; Madeleine Parent-Vachon[1]; Pascal Vachon[1]; Francis Beaudry[1]; *[1]Universite de Montreal, St-Hyacinthe, QC*

MP 765 **Cellular Precision for Infrared Laser Ablation Tissue Microproteomics**; Chao Dong[1]; Fabrizio Donnarumma[1]; Kelin Wang[1]; Kermit K. Murray[1]; *[1]Louisiana State University, Baton Rouge, LA*

MP 766 **Quantitative Proteomics of Tuberculosis Lung FFPE Tissue by SWATH Analysis**; Amon Suzuki[1]; Yasuhiro Hirano[1]; Mina Kawamura[1]; Akihiro Ishizu[2]; Susumu Y. Imanishi[1]; *[1]Meijo University, Nagoya, Japan; [2]Hokkaido University, Sapporo, Japan*

MP 767 **MS-Based Strategies Reveal Extracellular Matrix Alterations and N-Glycan Spatial Distribution Changes with the Progression of Ovarian Cancer**; Zihui Li[1]; Yatao Shi[2]; Fengfei Ma[2]; Kristal L. Gant[3]; Manish S. Patankar[3]; Lingjun Li[1,2]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [3]Department of Obstetrics and Gynecology, University of Wisconsin-Madison, Madison, WI*

MP 768 **Latest developments of Liquid Extraction Surface Analysis Mass Spectrometry for Top-Down and Bottom-Up Investigation of Protein Biomarkers in Renal Fibrosis**; Emma K Sisley[1]; Francisco Fernandez-Lima[2]; Tim Johnson[3]; Peter Hall[3]; Iain B Styles[1]; Helen J Cooper[1]; *[1]University of Birmingham, Birmingham, United Kingdom; [2]Florida International University, Miami, FL; [3]UCB Pharma LTD, Slough, United Kingdom*

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MP 769 **Large-Scale Qualitative and Quantitative Top-Down Proteomics Using Capillary Zone Electrophoresis-Electrospray Ionization-Tandem Mass Spectrometry with Nanograms of Proteome Samples**; Rachele Lubeckyj[1]; Abdul Rehman Basharat[2]; Xiaojing Shen[3]; Xiaowen Liu[2,4]; Liangliang Sun[3]; *[1]Michigan State University, East Lansing, MI; [2]Indiana University-Purdue University Indianapolis, Indianapolis, Indiana; [3]Michigan State University, East Lansing; [4]Indiana University School of Medicine, Indianapolis, Indiana*

MP 770 **Top-down Analysis of β-lactoglobulin Involving Disulfide Bond Cleavages**; Jianzhong Chen; *University of Alabama at Birmingham, Birmingham, AL*

MP 771 **Valet Parking for Protein Ion Charge State Concentration: Ion/Molecule Reactions in Linear Ion Traps**; David Foreman[1]; Jay Bhanot[1]; Kenneth W Lee[1]; Scott A McLuckey[1]; *[1]Purdue University, West Lafayette, IN*

MP 772 **Single Muscle Fiber Proteomics Enabled by High Sensitivity Top-Down Mass Spectrometry**; Jake A. Melby[1]; Yutong Jin[1]; Trisha Tucholski[1]; Yanlong Zhu[1]; Ziqing Lin[1]; Gary Diffee[1]; Ying Ge[1]; *[1]University of Wisconsin, Madison, Madison, WI*

MP 773 **Improved Top-Down Search Accuracy and Sensitivity using MetaMorpheus and a Novel Algorithm for Monoisotopic Mass Determination**; Robert Millikin[1]; Leah V. Schaffer[1]; Michael R. Shortreed[1]; Lloyd M. Smith[1]; *[1]University of Wisconsin Madison, Madison, WI*

MP 774 **Top-Down Proteomics Applied to Human CSF**; Marina Gay[1]; Ester Sánchez-Jiménez[1]; Laura Villarreal[1]; Mar Vilanova[1]; Romain Huguet[2]; Gianluca Arauz-Garofalo[1]; Antonio Lorenzo[1]; Mireia Díaz-Lobo[1]; Daniel López-Ferrer[2]; Marta Vilaseca[1]; *[1]Institute for Research in Biomedicine (IRB Barcelona), The Barcelona Institute of Science and Technology (BIST), Barcelona, Spain; [2]ThermoFisher, San Jose, CA*

MP 775 **Deciphering the Tubulin Code with Top-Down Proteomics**; Mathieu Dupré[1]; Thibault Chaze[1]; Elise Warter[2]; Serge Bonnefoy[2]; Jujimon A.s[3]; Philippe Bastin[2]; Carsten Janke[3]; Mariette Matondo[1]; Julia Chamot-Rooke[1]; *[1]Mass Spectrometry for Biology Unit, Institut Pasteur, CNRS USR2000, Paris, France; [2]Trypanosome Cell Biology Unit, Institut Pasteur, INSERM U1201, Paris, France; [3]Regulation of Microtubule Dynamics and Functions Unit, Institut Curie, CNRS UMR3348, Orsay, France*

MP 776 **Extending the Mass Range for Native Top-Down Mass Spectrometry by UVPD**; Jean-Francois Greisch[1,2]; Sem Tamara[1,2]; Albert J.R. Heck[1,2]; *[1]Biomolecular Mass Spectrometry and Proteomics, Bijvoet Center for Biomolecular Research and Utrecht Institute of Pharmaceutical Sciences, Utrecht University, Utrecht, Netherlands; [2]Netherlands Proteomics Center, Utrecht, Netherlands*

MP 777 **Controlling False-Discovery Rate for Top Down Proteomics Data Using UVPD Fragmentation**; Ken Durbin[1]; Luca Fornelli[2,3]; Joseph Greer[1]; Ryan Fellers[1]; Mick Greer[5]; David Horn[6]; Neil L Kelleher[3]; *[1]Proteinaceous, Evanston, IL; [2]University of Oklahoma, Norman, OK; [3]Northwestern University, Evanston, IL; [4]Proteinaceous, Inc., Evanston, IL; [5]Thermo Fisher Scientific, Austin, TX; [6]Thermo Fisher Scientific, San Jose, CA*

MP 778 **Precise Characterization and Comparison of KRAS Oncoproteoforms across Three Cancer Contexts**; Lauren Adams[1]; Caroline J DeHart[1]; Lissa C Anderson[2]; Luca Fornelli[3]; Christopher L. Hendrickson[2]; Neil L Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]National High Magnetic Field Laboratory, Tallahassee, FL; [3]University of Oklahoma, Norman, OK*

MP 779 **Large Scale Informatics for Interrogating Proteoforms in Human Blood Cells with Top Down Proteomics**; Joseph B Greer[1]; Ryan T Fellers[1]; Richard D Leduc[1]; Bryan P Early[1]; Josiah E Hutton[1]; Rafael D Melani[1]; Jacek W Sikora[1]; R Vince Gerbasi[1]; Jeannie M Camarillo[1]; Paul M Thomas[1]; Neil L Kelleher[1]; *[1]Northwestern University, Evanston, IL*

MP 780 **High-Field Asymmetric Ion Mobility Spectrometry of Heterogeneous Proteoform Populations from Primary Human Leukocytes**; Robert V Gerbasi[1]; Susan E Abbatiello[2]; Rafael D. Melani[1]; Michael W. Belford[3]; Scott M. Peterman[3]; Romain Huguet[3]; Philip D. Compton[1]; Paul M Thomas[1]; Neil L Kelleher[1]; *[1]Northwestern University, Evanston, IL; [2]Northeastern University, Boston, MA 02115; [3]Thermo Fisher Scientific, San Jose, CA*

MP 781 **Identification of Lactobacillus and Saccharomyces at Species Level in Industrial Ethanol Production Using Spectral Signatures by MALDI-TOF MS**; Juliana Guimarães Fonseca; *ESALQ/ USP, Piracicaba, Brazil*

MP 782 **Middle Down Approach for the Characterization of Monoclonal Antibodies after Ides Digestion and ETD Fragmentation**; John L. Snyder[1]; Colin M Wynne[1]; Michelle English[2]; Marshall Bern[2]; *[1]Eurofins Lancaster Laboratories, Inc., Lancaster, PA; [2]Protein Metrics Inc., San Carlos, CA*

MP 783 **Profiling Combinatorial Posttranslational Modifications in Seminal Plasma from Dairy Bulls *via* Sheathless Capillary Zone Electrophoresis – Top-Down Mass Spectrometry**; Fabio P. Gomes[1]; Jolene K. Diedrich[1]; Anthony J. Saviola[1]; Abdullah Kaya[2]; Erdogan Memili[3]; Arlindo A. Moura[4]; John R. Yates, III[1]; *[1]The Scripps Research Institute, La Jolla, CA; [2]Selcuk University, Selçuklu, Turkey; [3]The Mississippi State University, Starkville, MS; [4]The Federal University of Ceara, Fortaleza, Brazil*

MP 784 **Dipolar DC Induced Collisional Activation of Non-Dissociated Electron-Transfer Products**; Sarju Adhikari[1]; Mack Shih[1]; Eric T Dziekonski[2]; Frank A Londry[2]; Scott A McLuckey[1]; *[1]Purdue University, West Lafayette, IN; [2]SCIEX, Concord, ON*

MP 785 **Enhancing Top-Down Proteomics Data Analysis by Combining Deconvolution Results using Ensemble Methods**; Molly Wetzel[1]; Daniel Belongia[2]; Yutong Jin[3]; Zhijie Wu[3]; Irene M. Ong[2,4,5]; Sean J. McIlwain[1,4]; Ying Ge[1,2,6,7]; *[1]Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; [2]School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI; [3]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [4]Department of Biostatistics and Medical Informatics, University of Wisconsin - Madison, Madison, WI; [5]Department of Obstetrics & Gynecology, University of Wisconsin - Madison, Madison, WI; [6]Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706; [7]Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI*

MP 786 **Charge Deconvolution of Dissociation Spectra of Protein Complexes**; Marshall W. Bern[1]; Yong J. Kil[1]; Jing Yan[2]; Zachary L VanAernum[2]; Vicki H Wysocki[2]; *[1]Protein Metrics, San Carlos, CA; [2]The Ohio State University, Columbus, OH*

MP 787 **Investigation into Data-Independent Acquisition in Orbitrap and TOF platform for Topdown Proteomics Using Intact and Byonic software**; Victoria Sanchez[1]; Elisabeth Weyher[1]; K. Ilker Sen[2]; Marshall W. Bern[2]; Nagarjuna Nagaraj[1]; *[1]Max Planck Institute of Biochemistry, Martinsried, Germany; [2]Protein Metrics Inc., Cupertino, CA*



Set up all Tuesday posters
7:00 - 8:00 am

Odd-numbered posters present
10:30 - 11:30 am PLUS 12:30 – 2:30 pm

Even-numbered posters present
10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm

Remove all Tuesday posters
7:00 - 8:00 pm

Antibodies & Antibody Drug Conjugates I 001-022
Art, Archaeology & Paleontology 023-036
Biomarkers: Discovery I 037-068
Biomarkers: Quantitative Analysis II 069-099
Clinical Analysis II 100-123
Disease Biomarkers I 124-141
Energy: Hydrocarbon and Petrochemical 142-159
Environmental: General II 160-191
Environmental: Pharmaceuticals and Pesticides 192-212
Food Safety II 213-242
Forensics II 243-269
Fundamentals: Ion Structure/Energetics 270-287
Fundamentals: Ionization Mechanisms 288-297
GC/MS: Instrumentation and Applications I 298-318
H/D Exchange: Protein Structure/Function 319-343
Imaging MS: Method Development I 344-364
Imaging MS: Pharmaceutical Applications 365-379
Imaging MS: Sample Preparation 380-387
Imaging MS: Small Molecules 388-407
Imaging MS: Software 408-415
Informatics: Multiomics Integration 416-440
Instrumentation: Mini/Portable/Fieldable MS 441-457
Instrumentation: New Developments in Ion Detection 458-496
Ion Mobility: Applications I 497-519
Ion Mobility: FAIMS/DMS 520-529
Metabolomics: General I 530-549
Metabolomics: Untargeted Metabolite Profiling 550-568
Phosphopeptides: Quantitative Analysis 569-579
Protein Therapeutics: Quantitative Analysis II 580-605
Protein Therapeutics: Structural Characterization II 606-625
Proteins: PTMs I 626-646
Proteomics: Infectious Diseases 647-657
Proteomics: Intact Proteins 658-666
Proteomics: New Approaches I 667-694
Proteomics: Quantitative II 695-717
Proteomics: Top Down Analysis II 718-737
Small Molecules: Qualitative Analysis 738-756
Systems Biology 757-780

ANTIBODIES & ANTIBODY DRUG CONJUGATES I
001-022

TP 001 **Evaluating the Performance of an Orbitrap Tribrid at 8000 m/z**; John P. McGee[1]; Rafael Melani[1]; Mike Senko[2]; Vlad Zabrouskov[2]; Philip Remes[2]; Graeme McAlister[2]; Christopher Mullen[2]; Jesse Canterbury[2]; Michael Goodwin[2]; Romain Huguet[2]; Lee Early[2]; Neil L. Kelleher[1]; Philip D. Compton[1]; *[1]Northwestern University, Evanston, IL; [2]Thermo Fisher Scientific, San Jose, CA*

TP 002 **Analysis of Therapeutic Monoclonal Antibodies Using Volatile pH Gradient Cation Exchange Chromatography Directly Coupled to Native Mass Spectrometry**; Julia Baek[1]; Rosa Viner[2]; Terry Zhang[2]; James Ngai[3]; Eugen Damoc[4]; Shanhua Lin[5]; *[1]Thermo Fisher Scientific, Sunnyvale, California; [2]Thermo Fisher Scientific, San Jose, California; [3]Thermo Fisher Scientific, Sunnyvale; [4]Thermo Fisher Scientific, Bremen, Germany; [5]Thermo Fisher Scientific, Sunnyvale, CA*

TP 003 **Online IEX-MS Characterization and Monitoring of mAb Charge Heterogeneity Using an Optimized Cation Exchange Resin and Compact TOF Mass Spectrometer**; Samantha Ippoliti[1]; Qi Wang[1]; Ying Qing Yu[1]; Matthew A. Lauber[1]; Henry Shion[1]; *[1]Waters Corporation, Milford, MA*

TP 004 **Optimizing MS/MS Acquisition to Generate a Comprehensive Multi-Attribute Method Data Archive of the NISTmAb**; Michael E. Pettit[1]; John E. Schiel[1]; *[1]National Institute of Standards and Technology, Gaithersburg, MD*

TP 005 **A Novel Approach to Stability Characterization of ADC Payload Related Degradation through Assessment of Capped Drug-Linker ADC Surrogates**; Michael Lesslie[1]; Beijing Huang[1]; Gilbert Mbah[1]; Brittney Mills[1]; Jianwen Xu[2]; *[1]AbbVie Inc., North Chicago, IL; [2]AbbVie Inc., Worcester, MA*

TP 006 **Improve Sensitivity and Mass Accuracy in IEC-MS Analysis of Antibody Charge Variants**; Kyoung-Soon Choi[1]; Zhongping Liao[1]; Jason X. Tang[1]; *[1]Eli Lilly & Company, Indianapolis, IN*

TP 007 **Coupling Mixed-Mode Size Exclusion Chromatography with Native Mass Spectrometry for the Analysis of Intact Monoclonal Antibodies**; Yuetian Yan[1]; Tao Xing[1]; Shunhai Wang[1]; Ning Li[1]; Thomas J. Daly[1]; *[1]Regeneron, Tarrytown, NY*

TP 008 **Development and Qualification of a Difluoroacetic acid (DFA)-Based Subunit LC-MS Method for ADC Characterization**; Jacquelynn Smith[1]; Jennifer Nguyen[2]; Olga Friese[1]; Jason Rouse[3]; Matthew A. Lauber[2]; *[1]Pfizer, Chesterfield, MO; [2]Waters Corporation, Milford, MA; [3]Pfizer, Andover, MA*

TP 009 **Application of Wildcard Search Approach in Sequence Variant Analysis**; Yutian Gan; *Genentech, Inc., South San Francisco, CA*

TP 010 **EThcD Spectrum with Deep Novo Enables the Discrimination of Leucine and Isoleucine**; Yi Liu[1]; Wen Zhang[1]; Rui Qiao[2]; Ngoc Hieu Tran[2]; Lei Xin[1]; *[1]Bioinformatics Solutions Inc., Waterloo, ON; [2]University of Waterloo, Waterloo, ON*

TP 011 **A Simple Approach for Improved LC-MS Analysis of Protein Biopharmaceuticals *via* Modification of Desolvation Gas**; Shunhai Wang[1]; Tao Xing[1]; Anita P Liu[1]; Zehong He[1]; Yuetian Yan[1]; Thomas J Daly[1]; Ning Li[1]; *[1]Regeneron Pharmaceuticals Inc., Tarrytown, NY*

TP 012 **Characterization of Cetuximab using pH Gradient Cation Exchange and Microchip Electrophoresis Coupled to Native Orbitrap Mass Spectrometry**; Florian Fuessl[1]; Craig Jakes[1]; Sara Carillo[1]; Ashley Bell[2]; Erin A. Redman[2]; Ken Cook[3]; Jonathan Bones[1]; *[1]The National Institute for Bioprocessing Research & Training, Dublin, Ireland; [2]908 Devices, Boston, MA; [3]Thermo Fisher Scientific, Hemel Hempstead, UK, Hemel Hempstead, United Kingdom*



TP 013 **Analysis of Monoclonal Antibodies using SEC-MS in Native and Denaturing States to Identify Aggregation during DuoBody Formation**; Elsa Gorre[1]; Rajiv Rao[2]; Rebecca Smith[2]; Andrew Mahan[1]; Harsha Gunawardena[1]; Hirsh Nanda[1]; *[1]Janssen Research and Development, Spring House, PA; [2]Janssen Research & Development, Large Molecule Drug Product Development, Malvern, PA*

TP 014 **Structural Characterizations of Intact Monoclonal Antibodies by Native MS**; Angela Criscuolo[1, 2]; Tabiwang N. Arrey[2]; Eugen Damoc[2]; Thomas Moehring[2]; Catharina Crone[2]; Markus Kellmann[2]; *[1]Leipzig University, Leipzig, Germany; [2]Thermo Fisher Scientific (Bremen) GmbH, Bremen, Germany*

TP 015 **Automated Comprehensive Characterization and Quantification of Low-Abundance Sequence Variants in a Standard Monoclonal Antibody**; Joe Shambaugh[1]; Aude Tartiere[2]; Albert Van Wyk[3]; John McCarter[4]; Cassandra Wigmore[5]; Peter Haberl[6]; *[1]Genedata Inc, Lexington, MA; [2]Genedata, Inc., San Francisco, CA; [3]Genedata Ltd, Cambridge, United Kingdom; [4]Genedata, Inc., Lexington, MA; [5]Genedata AG, Basel, Switzerland; [6]Genedata GmbH, Munich, Germany*

TP 016 **Using Cation Exchange Chromatography and Online Mass Spectrometry (CEX-MS) for Assignment of iCIEF Charge Variants**; Kevin Ray[1]; Ben Cutak[1]; Shreya Ahuja[1]; *[1]MilliporeSigma, St. Louis, MO*

TP 017 **Characterization of BiTE® Antibody Constructs by Hydrophilic Interaction Chromatography Coupled to Mass Spectrometry**; Yang Stella Song[1]; Amy Huang[1]; John Harrahy[1]; *[1]Amgen Inc., Cambridge, MA*

TP 018 **Native Top-Down Analysis of Intact Antibodies Using Multiple Dissociation Techniques on a Tribrid Quadrupole Orbitrap Linear Ion Trap Mass Spectrometer**; Eugen Damoc[1]; Kristina Srzentić[2]; Romain Huguet[3]; Graeme McAlister[3]; Christopher Mullen[3]; Philip M Remes[3]; Jesse D Canterbury[3]; Mike Senko[3]; Vlad Zabrouskov[3]; *[1]Thermo Fisher Scientific, Bremen, Germany; [2]Thermo Fisher Scientific, Cambridge, Massachusetts; [3]Thermo Fisher Scientific, San Jose, California*

TP 019 **Process Monitoring of Monoclonal Antibodies at Intact and Subunits Levels using a Single Quadrupole LC/MS for Quality Control**; Linfeng Wu[1]; Lisa Zang[1]; Guannan Li[1]; *[1]Agilent Technologies, Santa Clara, CA*

TP 020 **The Impact of Using Different Protease Combinations for "de novo" Protein Sequencing**; Thierry Le Bihan[1]; Paul Taylor[1]; Zac McDonald[1]; Qixin Liu[1]; Jianqiao Shen[1]; Kathleen Gorospe[1]; Xin Xu[1]; Chris Hosfield[2]; Bin Ma[1, 3]; *[1]Rapid Novor Inc, Kitchener; [2]Promega Corporation, Madison, WI; [3]University of Waterloo, Waterloo*

TP 021 **Improving Assignment of Sequence Variants Using Machine Learning**; Sibylle Heidelberger[1]; Lyle Burton[2]; Sean L. Seymour[3]; *[1]AB Sciex UK Ltd, Warrington, United Kingdom; [2]SCIEX, Concord, ON; [3]Seymour Data Science, San Francisco, CA*

TP 022 **Isotope Selection in Label-Free Quantification and its Effects in Biopharmaceutical Characterization**; David Mahon[1]; K. Ilker Sen[2]; Yong J. Kil[2]; Promod Mehndiratta[1]; *[1]Celgene, Summit, NJ; [2]Protein Metrics Inc., Cupertino, CA*

ART, ARCHAEOLOGY & PALEONTOLOGY
023-036

TP 023 **What Sherlock Sorely Missed: The EVA Technology for Cultural Heritage Exploration**; Gleb Zilberstein[1]; Alfonsina D'Amato[2]; Piergiorgio Righetti[3]; *[1]Spectrophon Ltd,, Rehovot, Israel; [2]Università degli Studi di Milano, Dept. Pharmaceutical Sciences, Milano, Italy; [3]Politecnico di Milano, Dept. of Chemistry, Milano, Italy*

TP 024 **Multiple Techniques Confirm Collagen Remnants in Fossil Bone**; Brian Thomas[1]; Robert Layfield[2]; Lynn Smith[3]; Barry Shaw[2]; Stephen Taylor[4]; *[1]University of Liverpool, Glenn Heights, TX; [2]University of Nottingham, Nottingham, United Kingdom; [3]Norton Priory, Runcorn, United Kingdom; [4]Mass Spectometry Group, University of Liverpool, Liverpool, United Kingdom*

TP 025 **Palaeoproteomics on Paintings: Tandem Mass Spectrometry Unravels the History of Artistic Materials through Post-Translational Modifications**; Fabiana Di Gianvincenzo[1]; Meaghan Mackie[1, 2]; Patrick Rüther[2]; Diana Samodova[2]; David Peggie[3]; Jesper V. Olsen[2]; Enrico Cappellini[1]; *[1]Department of Biology, University of Copenhagen, Copenhagen, Denmark; [2]NNF Center for Protein Research University of Copenhagen, Copenhagen, Denmark; [3]National Gallery of London, London, United Kingdom*

TP 026 **Identification of Animal Species by Mass Spectrometry of Collagen Extracted from Neolithic and Paleolithic Bones and Teeth**; Takashi Nakazawa[1]; Momoko Osawa[1]; Kana Matsuo[1]; Mako Inuzuka[1]; Yuki Ito[1]; Kazuki Kawahara[2]; Yuichi Naito[3]; Seiji Kadowaki[3]; Yoshihiro Nishiaki[4]; *[1]Nara Women's University, Nara, Japan; [2]Osaka University, Suita, Japan; [3]Nagoya University, Nagoya, Japan; [4]The University of Tokyo, Bunkyo, Japan*

TP 027 **Species Identification of Materials Used in Cultural Heritage Objects from Alaska in the British Museum's Collection Using 'ZooMS' Methodology**; Michael Douglas Nairn[1]; Chris Mussell[2]; Amber Lincoln[2]; *[1]Shimadzu, Manchester, UK, Manchester, United Kingdom; [2]The British Museum, London, United Kingdom*

TP 028 **GrandPep, a Novel Software for Computational Reconstruction of Ancient Protein Sequences**; Petra Gutenbrunner[1]; Frido Welker[2]; Jazmin Ramos Madrigal[2]; Enrico Cappellini[2]; Juergen Cox[1]; *[1]Max-Planck Institute of Biochemistry, Planegg, Germany; [2]Department of Biology, University of Copenhagen, Copenhagen, Denmark*

TP 029 **Effects of Preparation Methods, Environmental Factors, and Scientific Analysis on Aging of Historical Silk, Parchment, and Bone at Molecular Levels**; Mehdi Moini; *George Washington University, Washington, VA*

TP 030 **Revealing the Past through Non-invasive Metabolomics and Proteomics**; Elettra Barberis[1]; Marcello Manfredi[2]; Pier Giorgio Righetti[3]; Gleb Zilberstein[4]; Bianucci Raffaella[5]; Emilio Marengo[2]; *[1]University of Piemonte Orientale - Department of Sciences and Technological Innovation, Alessandria, Italy; [2]University of Piemonte Orientale, Alessandria, Italy; [3]Politecnico di Milano, Dept. of Chemistry, Milano, Italy; [4]Spectrophon Ltd,, Rehovot, Israel; [5]University of Turin, Torino, Italy*

TP 031 **Microwave-Assisted Acid Hydrolysis for Whole Bone Proteomics and Paleoproteomics**; Caitlin Colleary[1]; Timothy P Cleland[1]; *[1]Smithsonian Museum Conservation Institute, Suitland, MD*

TP 032 **Archival Proteins: Biomolecular Evidence of Parchment Production Methods**; Carla L Soto Quintana[1]; Sarah Fiddyment[1]; Matthew J Collins[2, 3]; *[1]University of York, York, United Kingdom; [2]University of Copenhagen, Copenhagen, Denmark; [3]University of Cambridge, Cambridge, United Kingdom*

TP 033 **Robust Proteomics Workflow for the Identification and Classification of Paleontological Bones**; Fabrice Bray[1]; Stéphanie Flament[1]; Patrick Auguste[1]; Christian Rolando[1]; *[1]Université de Lille, Villeneuve d'Ascq, France*

TP 034 **Digging Deeper into Ancient Proteomes – Improved Sampling and Instrumentation Allow for an Unprecedented View of the Archaeological Protein Record**; Patrick L. Ruether[1]; Alberto J. Taurozzi[2]; Dorte B. Bekker-Jensen[1]; Tanveer S. Batth[1]; Tabiwang N. Arrey[3]; Alexander Harder[3]; Christian D. Kelstrup[1]; Enrico Cappellini[2]; Jesper V. Olsen[1]; *[1]NNF Center for Protein*

Research University of Copenhagen, Copenhagen, Denmark; [2]Natural History Museum of Denmark, Copenhagen, Denmark; [3]Thermo Fisher Scientific, Bremen, Germany

TP 035 **Multidisciplinary Approach to Understanding Preservation and Decomposition at Vindolanda, Roman Fort, UK**; gillian Taylor[1]; Hrafnhildur Helga Halldórsdóttir[1]; Rhys Williams[1]; Caroline Orr[1]; Andrew Birley[2]; *[1]Teesside University, Middlesbrough, United Kingdom; [2]Vindolanda, Bardon Mill, United Kingdom*

TP 036 **Adapting Historic Architecture and Engineering Documentation Protocols to the Virtual Preservation of Historically Important Analytical Instruments**; Frances R. Gale[1]; P. Jane Gale[2]; Michael A Grayson[3]; *[1]University of Texas at Austin School of Architecture (ret), Austin, TX; [2]ASMS Archivist/Historian, Southborough, MA; [3]ASMS Archivist/Historian (ret), St. Louis, MO*

BIOMARKERS: DISCOVERY I
037-068

TP 037 **Coccidioidomycosis Detection Using Targeted Plasma and Urine Metabolic Profiling**; Paniz Jasbi[1]; Natalie M. Mitchell[2]; Xiaojian Shi[1]; Thomas E. Grys[3]; Yiping Wei[1]; Li Liu[2,4]; Douglas F. Lake[2]; Haiwei Gu[1]; *[1]Arizona State University, Phoenix, AZ; [2]Arizona State University, Tempe, AZ; [3]Mayo Clinic, Phoenix, AZ; [4]Mayo Clinic, Scottsdale, AZ*

TP 038 **Quantitative Serum Proteomics Uncovers Biomarkers for the Prediction of *Staphylococcus aureusbacteremia* Patient Outcomes and Highlights Dysregulated Host Defense Networks**; Jacob Wozniak[1]; Warren Rose[2]; George Sakoulas[1]; David J Gonzalez[1]; *[1]UCSD, San Diego, CA; [2]University of Wisconsin, Madison, Madison, WI*

TP 039 **Proteomic and Lipidomic Analysis Reveals Altered Fatty Acid Metabolism in the Liver of the Symptomatic Niemann-Pick, Type C1 Mouse Model**; Melissa R Pergande[1]; Jonathon Hanek[1]; Estefania Zárate[1]; Sheher Banu Mohsin[2]; Carol Haney-Ball[3]; Stephanie M Cologna[1]; *[1]University of Illinois at Chicago, Chicago, IL; [2]Agilent Technologies, Wood Dale, IL; [3]Agilent Technologies, Cary, NC*

TP 040 **Epitope Structures of Aptamer Complexes of the Multi-domain Protein C-Met Revealed by Proteolytic Affinity-Mass Spectrometry**; Michael Przybylski[1]; Loredana Lupu[2]; Pascal Wiegand[2]; Nico Hüttmann[2]; Stephan Rawer[2]; Wolfgang Kleinekofort[2,3]; Irina Shchugoreva[4]; Anna S. Kichkailo[5]; Felix N. Tomilin[4]; Alexander Lazarev[6]; Maxim V. Berezovski[7]; *[1]Steinbeis Centre Biopolymer Analysis and Biomedical Mass Spectrometry, Ruesselsheim, Germany; [2]Steinbeis Centre Biopolymer Analysis and Biomedical Mass Spectrometry, Ruesselsheim, Germany; [3]Rhein Main University, Rüsselsheim, Germany; [4]Kirensky Institute of Physics, Russian Academy of Sciences, Krasnoyarsk, Russia; [5]Krasnoyarsk State Medical University, Krasnoyarsk, Russia; [6]Pressure Biosciences Inc., South Easton, MA; [7]University of Ottawa, Dept. Chemistry, Ottawa, Quebec*

TP 041 **Novel S-Nitrosylated Proteolytic Peptides Derived from Postsynaptic Proteins for Alzheimer's Disease**; George Anis Sarkis[1]; John S. Wishnok[1]; Steven R Tannenbaum[1]; *[1]Massachusetts Institute of Technology, Cambridge, MA*

TP 042 **High-Throughput Screening of Antimicrobial Resistance by MALDI-High Resolution Mass Spectrometry of Bacterial Cell Cultures**; Evan Larson[1]; Andrew Petersen[1]; Bryan Bellaire[1]; Young Jin Lee[1]; *[1]Iowa State University, Ames, IA*

TP 043 **Targeted Metabolomics Profile Sow Milk Components by LC-MS/MS**; Shen Allison[1]; Qisheng Zhong[2]; *[1]Shimadzu Global COE, Shimadzu (China) Co., Ltd., China, Guangzhou, China; [2]Shimadzu Global COE, Shimadzu (China) Co., Ltd., China, Guangzhou, China*

TP 044 **Colorectal Cancer Patient-Derived Serum Exosomes Promote Cancer Cell Migration**; Hye Ryeon Jung[1]; Yu-Ri Seo[1]; Jeehee Park[1]; Eugene C. Yi[1]; *[1]Department of Molecular Medicine and Biopharmaceutical Sciences, Graduate School of Convergence Science and Technology, Seoul National University, Seoul, South Korea*

TP 045 **Identification of Novel Serum Protein Biomarkers for ALS Diagnosis and Progression**; Szymon Filip[1]; Tori Sosnowski[1]; Halil Idrisoglu[2]; Hande Ozdinler[3,4]; Young Ah Goo[1]; *[1]Proteomics Center of Excellence, Northwestern University, Chicago, IL; [2]Istanbul University, Istanbul, Turkey; [3]Department of Neurology, Northwestern University, Feinberg School of Medicine, Chicago, IL; [4]Les Turner ALS Center at Northwestern University, Chicago, IL*

TP 046 **Identifying Peptide Signatures in Longitudinally Collected CSF Associated with Progression of ALS Using DIA Mass Spectrometry**; Allyson L Mellinger[1]; Jeffrey R. Enders[2]; Michael S. Bereman[1,3,4]; *[1]Department of Chemistry, North Carolina State University, Raleigh, NC; [2]Molecular Education, Technology, and Research Innovation Center, Raleigh, NC; [3]Center for Human Health and the Environment, North Carolina State University, Raleigh, NC; [4]Department of Biological Sciences, North Carolina State University, Raleigh, NC*

TP 047 **Lipid Biomarker Identification for Preterm Birth and Miscarriage *via* Deuterium Oxide Labeling for Global Omics Relative Quantification**; Byoungsook Goh[1]; Ji-Yeon Park[2]; Joo-Hee Choi[2]; Jong-Hwan Park[2]; Tae-Young Kim[1,3]; *[1]Department of Chemistry, Gwangju Institute of Science and Technology, Gwangju, South Korea; [2]Laboratory Animal Medicine, College of Veterinary Medicine and BK 21 PLUS Project Team, Chonnam National University, Gwangju, South Korea; [3]School of Earth Sciences and Environmental Engineering, Gwangju Institute of Science and Technology, Gwangju, South Korea*

TP 048 **An Integrated System for Sequential Isolation of Circulating Tumor Cells and Exosomes for Proteomic Analysis from the Same Blood Sample**; Jie Zhang[1]; Jianhui Zhu[1]; Zhijing Tan[1]; Mingrui An[1]; Yingfeng Zhang[1]; Neehar D. Parikh[1]; David M. Lubman[1]; *[1]University of Michigan Medical Center, Ann Arbor, MI*

TP 049 **Screening of Site-Specific Glycopeptides in Serum Haptoglobin as Novel Biomarkers for Non-Alcoholic Steatohepatitis Using EThcD-MS/MS**; Jianhui Zhu[1]; Jie Zhang[1]; Zhengwei Chen[2]; Gabriela Grigorean[3]; Lingjun Li[2]; David M. Lubman[1]; *[1]University of Michigan Medical Center, Ann Arbor, MI; [2]University of Wisconsin-Madison, Madison, WI; [3]University of Michigan, Ann Arbor, MI*

TP 050 **Systematic Proteomic Analysis of the interaction between UPR and LPS regulated Phosphorylation Establishes Novel Connections to Innate Immunity**; Min Ma[1]; Yatao Shi[1]; Yusi Cui[1]; Junfeng Huang[1]; Yiping Liu[1]; Judith A Smith[1]; Lingjun Li[1]; *[1]University of Wiscision-madison, WI*

TP 051 **Establishment of Q-markers of Niaoduqing Granule by High Resolution Mass Spectrum Analysis and Network Pharmacology Study**; Yi-Sheng Xu[1]; Yuanyuan Xie[2]; *[1]waters cooperation, Shanghai, China; [2]Tsinghua University, Beijing, China*

TP 052 **Effects of Daily Vinegar Ingestion on Insulin Sensitivity, Visceral Fat, Body Weight and the Metabolome in Healthy Adults**; Paniz Jasbi[1]; Olivia Baker[2]; Xiaojian Shi[1]; Lisa Gonzalez[2]; Summer Anderson[2]; Xinchen Wang[1]; Haiwei Gu[1]; Carol S. Johnston[2]; *[1]Arizona State University, Scottsdale, AZ; [2]Arizona State University, Phoenix, AZ*

TP 053 **Lipidomics of Parkinson's Disease: Towards More Accurate Diagnosis Methods through Omics Technologies**; Adriana Zardini Buzatto[1]; Barinder Bajwa[1]; Jaspaul Tatlay[1]; Roger A Dixon[1]; Richard Camicioli[1]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB*



TP 054 **Ovarian Cancer Detection Using Plasma Metabolic Profiling**; Yiping Wei[1]; Paniz Jasbi[1]; Xiaojian Shi[1]; Haiwei Gu[1]; *[1]Arizona State University, Scottsdale, AZ*

TP 055 **Mapping and Sequencing of Gangliosides in Human Cerebellum at Different Developmental Stages by Orbitrap Multistage Mass Spectrometry**; Raluca Ica[1]; Mirela Sarbu[1]; Alina Petrut[1]; Cristian VA Munteanu[2]; Andrei J Petrescu[2]; Radu Albulescu[3]; Alina D. D Zamfir[1]; *[1]National Institute for Research and Development in Electrochemistry and Condensed Matter, Timisoara, Romania, Timisoara, Romania; [2]Institute of Biochemistry of the Romanian Academy, Bucharest, Romania; [3]National Institute for Chemical - Pharmaceutical Research and Development, Bucharest, Romania*

TP 056 **Lipidomics of Alzheimer's Disease and Cerebral Amyloid Angiopathy: Identification of Potential Biomarkers in Human Plasma by UHPLC-MS**; Barinder Bajwa[1]; Adriana Zardini Buzatto[1]; Roger A Dixon[1]; Richard Camicioli[1]; Eric E Smith[2]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB; [2]University of Calgary, Calgary, AB*

TP 057 **Tyrosine Aminoacyl-tRNA Synthetase Sensitize Breast Cancer to the Combined Chemotherapeutic Regimen**; Ji hye Moon[1]; Dohyun Han[1]; Hyeyoon Kim[1]; Han Suk Ryu[1]; *[1]Seoul National University Hospital, Seoul, South Korea*

TP 058 **Development and Technical Validation of a Data-Independent Acquisition Approach for Analysis of Human Alzheimer's Disease Cerebrospinal Fluid**; Shannon N. Leslie[1]; Rashaun S. Wilson[2]; Pia W. Kivisakk[3]; Savannah E. Kandigian[3]; Bianca A. Trombetta[3]; Becky C. Carlyle[3]; Steven E. Arnold[3]; Angus C. Nairn[1]; *[1]Yale University, New Haven; [2]Yale University Keck MS & Proteomics Core, New Haven, CT; [3]Massachusetts General Hospital, Boston, Massachusetts*

TP 059 **Scalable and Automated Plasma Workflow Based on the Thermo Scientific Q Exactive HF-X MS platform**; Jing Wang[1]; Sarah Trusiak[1]; Ryan D. Bomgarden[2]; Sergei Snovida[3]; Emily I. Chen[1]; *[1]Thermofisher Scientific Precision Medicine Science Center, Cambridge, MA; [2]ThermoFisher Scientific, Rockford, IL; [3]Thermo Fisher Scientific, Rockford, IL*

TP 060 **Proteomic Characterization of the Warburg Effects in Clear Cell Renal Cell Carcinoma**; Yuling Chen[1]; Yang Lv[2]; Songfeng Wu[3]; Jiatong Xu[1]; Di Wu[2]; Haiteng Deng[1]; *[1]Tsinghua University, Beijing, China; [2]Center of Nephrology, the General Hospital of the PLA, Beijing, China; [3]Academy of Military Medical SciencesCountermeasures, Beijing, China*

TP 061 **Development of an LC-MRM-MS assay for Analysis of Prostate-Specific Antigen Including its Major Glyco-Proteoforms**; Yuri E.M. van der Burgt[1]; Kasper Siliakus[1]; Guinevere S.M. Lageveen-Kammeijer[1]; Manfred Wuhrer[1]; L. Renee Ruhaak[1]; Christa M. Cobbaert[1]; *[1]Leiden University Medical Center, Leiden, Netherlands*

TP 062 **A Highly Sensitive FFPE Tissue Workflow by Coupling the Micro Pillar Array Column (µPACTM) with High Resolution Mass Spectrometry**; Antonius Koller[1]; Sarah Trusiak[2]; Xinyu Zhang[2]; Alexander R Ivanov[1]; Emily I. Chen[2]; *[1]Northeastern University, Boston, MA; [2]Thermo Fisher Precision Medicine Science Center, Cambridge, MA,*

TP 063 **A Quantitative Proteomics Platform for Identifying Potential Biomarkers for Controlling Krypton Misuse in Horseracing**; Kin-Sing Wong[1]; Hiu Wing Cheung[1]; Timmy L.S. Choi[1]; Wai Him Kwok[1]; Terence S.M. Wan[1]; Jenny K.Y. Wong[1]; Peter Curl[2]; Stewart C. Mechie[2]; Anil Prabhu[2]; Emmie N.M. Ho[1]; *[1]Racing Laboratory, The Hong Kong Jockey Club, Hong Kong, Hong Kong; [2]Department of Veterinary Regulation & Biosecurity Policy, The Hong Kong Jockey Club, Hong Kong, Hong Kong*

TP 064 **Mass Spectrometric Analysis of Sebum Contents for Classification of Parkinson's Disease**; Drupad Trivedi[1]; Eleanor Sinclair[1]; Depanjan Sarkar[1]; Joy Milne[1]; Monty Silverdale[1]; Tilo Kunath[2]; Roy Goodacre[3]; Perdita Barran[1]; *[1]University of Manchester, Manchester, United Kingdom; [2]University of Edinburgh, Edinburgh, United Kingdom; [3]University of Liverpool, Liverpool, United Kingdom*

TP 065 **Proteomics Comparative Study of Exosome Subpopulations**; Yingfeng Zhang[1]; Jianhui Zhu[2]; Zhijing Tan[2]; David M. Lubman[3]; *[1]University of Michigan, ANN ARBOR, MI; [2]University of Michigan, Ann Arbor, Michigan; [3]University of Michigan, Ann Arbor, MI*

TP 066 **Protein Identification - the Translational Research Study of HBx Genes Related to Hepatocellular Carcinoma**; Ming-Hui Yang[1]; Yi-Ming Arthur Chen[2]; Yi-Chia Lee[3]; Yu-Chang Tyan[3]; *[1]National Health Research Institutes, Zhunan, Taiwan; [2]Taipei Medical University, Taipei, Taiwan; [3]Kaohsiung Medical University, Kaohsiung, Taiwan*

TP 067 **Use of untargeted metabolomics approach using label free LC-DIA-MS method to identify putative biomarkers involved in spontaneous pre-term birth (sp-PTB)**; Shirish Yakkundi[1]; James Langridge[2]; Lee A Gethings[2]; *[1]INFANT Centre, University College Cork, Cork, Ireland; [2]Waters Corporation, Wilmslow, United Kingdom*

TP 068 **Development of a Simple and Robust LC-MS/MS Method for the Quantification of the Renal Failure Biomarker Symmetric Dimethyl Arginine (SDMA)**; Brittany J Perley[1]; Alyssa Kabat[1]; Jem Sibbick[1]; Rachel Van Heest[1]; Sean Maki[1]; Katherine Henry[1]; Steven Wiltshire[1]; Allysen Meymaris[1]; *[1]Charles River Laboratories, Worcester, MA*

BIOMARKERS: QUANTITATIVE ANALYSIS II
069-099

TP 069 **Evaluation on LC-MS/MS Assay Using Anti-Peptide Immunocapture to Quantify PD-L1 As a Clinical Biomarker in FFPE Tissues for Immuno-Therapy Development**; Naiyu Zheng[1]; Kristin Taylor[1]; Huidong Gu[1]; Rasa Santockyte[1]; Xi-Tao Wang[1]; Yan J. Zhang[1]; Renuka Pillutla[1]; Jianing Zeng[1]; *[1]Bristol-Myers Squibb Company, Princeton, NJ*

TP 070 **Multiple Reaction Monitoring (MRM) and Parallel Reaction Monitoring (PRM) to Identify Biomarkers Predictive of Clinical Response to Tocilizumab (anti-IL-6) Treatment**; Jin woo Jung[1]; Byoung-Kyu Cho[1]; Kang Hyun Kim[1]; Yeong Wook Song[1,2]; Eugene C. Yi[1]; *[1]Department of Molecular Medicine and Biopharmaceutical Sciences, Graduate School of Convergence Science and Technology, Seoul National University, Seoul, South Korea; [2]Division of Rheumatology, Department of Internal Medicine, College of Medicine, Seoul National University, Seoul, South Korea*

TP 071 **Simultaneous Quantitation of Epinephrine and Norepinephrine as Cardiovascular Biomarkers in Rodent Species Plasma Utilizing a Non-Derivatized UHPLC-MS/MS Assay**; Craig Titsch[1]; Enzo Kandoussi[1]; Jianing Zeng[1]; Glen Banks[2]; Gayani Fernando[2]; Yan J. Zhang[1]; Renuka Pillutla[1]; Naiyu Zheng[1]; *[1]Bristol-Myers Squibb Co., Lawrenceville, NJ; [2]Bristol-Myers Squibb Co., Hopewell, NJ*

TP 072 **In-Sample Calibration Curve Using Multiple Isotopologue Reaction Monitoring of a SIL-Analyte for Instant LC-MS/MS Analysis of Biomarker and Quantitative Proteomics**; Huidong Gu[1]; Yue Zhao[1]; Marissa DeMichele[1]; Naiyu Zheng[1]; Yan J. Zhang[1]; Renuka Pillutla[1]; Jianing Zeng[1]; *[1]Bristol-Myers Squibb, Princeton, NJ*

TP 073 **Quantification of Soluble MERTK in Serum Using Affinity Enrichment-Liquid Chromatography Mass Spectrometry**; Yongxin Zhu[1]; Petia Shipkova[2]; Thomas Spires[2]; Karen Augustine[2]; Timothy Olah[2]; *[1]Bristol-Myers*

Squibb Company, Princeton, NJ; [2]Bristol-Myers Squibb Co., Princeton, NJ

TP 074 **Optimized high-throughput proteomic sample preparation in 96-well plate format for identifying serum Biomarkers of alpha-Dystroglycanopathy**; Mahmud Hossain[1]; Monica Lane[1]; Hongge Wang[1]; Jun Luo[1]; Bailin Zhang[1]; *[1]Sanofi Genzyme, Framingham, MA*

TP 075 **Urinary Mercapturic Acids of Volatile Organic Compounds and Oxidative/Nitrosative Stress Markers in Workers of the Semiconductor Industry**; Hsin-Chang Chen[1]; Chen-Hsien Lee[2]; Kai-Chieh Yang[1]; Wei-Lun Su[1]; Tzu-Sheng Fang[1]; Yi-Chen Sun[1]; *[1]Institute of Food Safety and Health, National Taiwan University, Taipei, Taiwan; [2]Institute of Labor, Occupational Safety and Health, Ministry of Labor, New Taipei City, Taiwan*

TP 076 **Multiplexed Detection of Biomolecules with High Sensitivity and Specificity Using Surface Mass Spectrometry**; Hee-Kyung Na[1, 2]; Hyun Kyong Shon[1]; Sunho Joh[1, 3]; Jeong-Hee Moon[4]; Hye Young Son[5]; Yong-Min Huh[5]; Tae Geol Lee[1]; *[1]KRISS, Daejeon, South Korea; [2]Seoul national university, Seoul, South Korea; [3]Department of Nano Science, University of Science and Technology, Daejeon, South Korea; [4]KRIBB, Daejeon, South Korea; [5]Department of Radiology, College of Medicine, Yonsei University, Seoul, South Korea*

TP 077 **Resolution and Quantitative Analysis of Human Urinary Isomeric Mercapturic Acids Derived from Crotonaldehyde, 2-Methylacrolein, and Methylvinyl Ketone**; Menglan Chen[1]; Steven Carmella[2]; Stephen S Hecht[2]; *[1]Masonic Cancer Center, U of MN, Minneapolis; [2]University of Minnesota, Minneapolis, MN*

TP 078 **Development of an Automated Sample Preparation Platform for cPILOT**; Albert Arul[1]; Renã A.S. Robinson[1]; *[1]Vanderbilt University, Nashville, TN*

TP 079 **Effect of Maternal Urinary and Placenta Melamine Levels during Pregnancy on Neonatal Birth Weight by Isotope Dilution LC-MS/MS**; Sih-Syuan Li[1]; Chung-Yi Huang[1]; Yung-Hung Chen[2]; Chia-Fang Wu[1]; *[1]Research Center for Environmental Medicine, Kaohsiung Medical University, Kaohsiung, Taiwan; [2]Department of Gynecology and Obstetrics, Kaohsiung Medical University Hospital, Kaohsiung Medical University, Kaohsiung, Taiwan*

TP 080 **Measurement of Cyclooxygenase Inhibition and Selectivity in Human Whole Blood Assay Using LC-MS/MS**; Yifan Shi[1]; Heather Murrey[1]; Kay Ahn[1]; Naidong Weng[1]; Shefali Patel[1]; *[1]Janssen, Spring House, PA*

TP 081 **Highly Sensitive Immuno-MRM Assay for Quantitation of PTEN in Both FFPE and Fresh Frozen Tissue**; Sahar Ibrahim[1]; Rene Zahedi[2]; Naciba Benlimame[3]; Adriana Aguilar[4]; Mark Basik[5, 6]; Gerald Batist[6, 7, 8, 9, 10]; Christoph H. Borchers[2, 11, 12, 13]; *[1]Department of Experimental Medicine, McGill University, Montreal, Québec; [2]Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; [3]Research Pathology Facility, Lady Davis Institute, Jewish General Hospital, McGill University, Montreal, QC; [4]Cancer Genomics and Translational Research Laboratory, Segal Cancer centre, Lady Davis Institute, McGill university, Montreal, QC; [5]Department of Medicine, Division of Experimental Medicine, McGill University, Montreal, QC; [6]Department of Oncology, McGill University, Montreal, QC; [7]Departments of Medicine and Oncology, McGill University, Montreal, QC; [8]Dept. of Oncology, Sir Mortimer B. Davis-Jewish General Hospital, Montreal, QC; [9]Segal Cancer Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, Montreal, QC; [10]McGill Centre for Translational Research in Cancer, Segal Cancer Centre / Lady Davis Institute, Jewish General Hospital, Montreal, QC; [11]University of Victoria-Genome BC Proteomics Centre, Victoria, BC; [12]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; [13]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC*

TP 082 **Rapid Profiling and Quantification of 17 Bile Acids in Human Plasma by LC-MS/MS**; Dan Li[1]; Frances Carroll[1]; Shun-Hsin Liang[1]; Ravali Alagandula[1]; Justin Steimling[1]; Sue Steinike[1]; Paul Connolly[1]; *[1]Restek, Bellefonte, PA*

TP 083 **Immunoaffinity LCMS Assay for Measuring Soluble B-Cell Maturation Antigenin Multiple Myeloma Patients**; Ying Zhang[1]; John K Meissen[1]; Kyle Wald[1]; Angela Stauffer[2]; Michael Hall[2]; Matthew Blatnik[1]; *[1]Pfizer Inc., Groton, CT; [2]Pfizer WRD, La Jolla, CA*

TP 084 **Development of LC-MS/MS Assays to Measure Thyroid Hormones in Rat Serum**; Hua Wang[1]; Seth R Bell[1]; Junhong Guo[1]; Jeroen Kooistra[1]; Pragati S Coder[1]; Liam B Moran[1]; Elizabeth A Groeber[1]; *[1]Charles River Laboratories, Ashland, OH*

TP 085 **Quantification of EDB+FN Levels in PDX Tumor and PDX FFPE Samples Using LC-MS/MS Methods**; Fengping Li[1]; Bing Kuang[2]; Andrea Hooper[3]; Jonathon Golas[3]; Chao-Pei Betty Chang[3]; Mauricio Leal[3]; Hendrik Neubert[1]; Lindsay King[1]; *[1]Pfizer, Andover, MA; [2]Pfizer WRD, La Jolla, California; [3]Pfizer WRD, Pearl River, New York*

TP 086 **Determining Isocyanate Exposure in Human Urine by LC-MRM**; Maggy Lepine[1, 2]; Lekha Sleno[1]; Jacques Lesage[1]; Sebastien Gagne[2]; *[1]UQAM, Montreal, QC; [2]IRSST, Montreal, QC*

TP 087 **Multiplexed Quantitative Glycoproteomic and Proteomic Analyses of Cerebrospinal Fluid in Alzheimer's Disease**; Xiaofang Zhong[1]; Zhengwei Chen[1]; Qinying Yu[1]; Henrik Zetterberg[2]; Cynthia Carlsson[1]; Ozioma Okonkwo[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI; [2]University of Gothenburg, Gothenburg, Sweden*

TP 088 **Quantification of Jag1 Protein in Agarose Inflated Lung Airway Samples by Immuno Affininty Enrichment and LC-MS/MS analysis**; Omar S. Barnaby[1]; Joon Nam[2]; Deanna Mohn[1]; Brian Bennet[2]; Jonathan Phillips[2]; Christopher A. James[1]; *[1]Amgen, Inc., Thousand Oaks, CA; [2]Amgen, Inc., Thousand Oaks, CA*

TP 089 **LC-MS/MSAnalysis of Arachidonic Acid as a Biomarker in Human Plasma for Clinical Studies**; Tian-Sheng Lu[1]; Elise Snider[1]; Nicole Greer[1]; Joshua Froning[1]; Yong-Xi Li[1]; *[1]Medpace Bioanalytical Laboratories, Cincinnati, OH*

TP 090 **Developing Protein Biomarker MRM Methods as an Alternative Indicator of Prohibited Substance Abuse in Equine Athletes**; Sophie Bromilow[1]; Heather Knych[1]; Ben Moeller[1]; Rick Arthur[1]; Claudia P.B. Martins[2]; David Horohov[3]; Scott Stanley[3]; *[1]K.L. Maddy Equine Analytical Chemistry Laboratory, Davis, CA; [2]ThermoFisher, San Jose, CA; [3]Gluck Equine Research Centre, Lexington, KY*

TP 091 **Metabolic Reprogramming in Prostate Cancer Cell Lines in Response to Tyrosine Kinase Inhibition**; Robert Sprung[1]; Surbhi Chouhan[1]; Petra Erdmann-Gilmore[1]; Qiang Zhang[1]; Rose Connors[1]; Yiling Mi[1]; Nupam Mahajan[1]; Reid Townsend[1]; *[1]Washington University, School of Medicine, St. Louis, MO*

TP 092 **Quantitative Measurement of 7-Ketocholesterol and Cholestane-3β,5α,6β-triol as Biomarkers in Human Serum Using LC-MS/MS**; Aiping Zhu[1]; Idana Santiago[1]; Yu Zhang[1]; Yong-Xi Li[1]; *[1]Medpace Bioanalytical Laboratories, Cincinnati, OH*

TP 093 **Dried Blood Spots from Frozen Whole Blood Provide an Option to Analyze Parkinson's Disease Cohorts for Activity of Lysosomal Enzymes**; Pavlina Wolf[1]; Roy Alcalay[2]; Karolina Helesicova[1]; Ruby Chiang[1]; Emma-Jane Turton[1]; Michael Pauciulo[3]; William Nichols[3]; Wendy Chung[4]; Pablo Sardi[1]; Kate Zhang[1]; Petra Oliva[1]; *[1]Sanofi, Framingham, MA; [2]Columbia University Medical Center, Neurological Institute, New York, NY; [3]Division of Human Genetics, Cincinnati Children's Hospital Medical Center*

and the Department of Pediatrics, University of Cincinnati College of Medicine, Cincinnati, OH; [4]Department of Pediatrics and Medicine, Columbia University Medical Center, New York, NY

TP 094 **LC-MS/MS Assay for Non-Invasive Detection of Prostaglandins and Leukotrienes in Urine**; Xiongfei Wu[1]; Hanjiao Song[1]; Weiqun Cao[1]; Lili Xing[1]; Xin Zhang[1]; Yi Tao[1]; *[1]WuXi AppTec, Shanghai, China*

TP 095 **Multiplexed Quantification of Sepsis Prognosis Candidate Biomarkers Spanning a Wide Dynamic Range of Plasma Concentrations (ng/ml to mg/ml)**; Christelle Dubois[1]; Didier Payen[2]; Stéphanie Simon[1]; François Fenaille[1]; Christophe Junot[1]; Nathalie Morel[1]; Francois Becher[1]; *[1]CEA Saclay, DRF, Institut Joliot, Service de Pharmacologie et d'Immunoanalyse- CEA-INRA UMR 0496, Laboratoire d'Etude du Métabolisme des Médicaments, Gif-sur-Yvette, France; [2]Department of Anesthesiology and Critical Care, Lariboisière Hospital, University of Paris Denis Diderot 7, Paris, France*

TP 096 **Metaproteomics of the Human Intestinal Microbiota in Physiological and Pathological Conditions**; celine Henry[1]; Ariane Bassignani[2,3]; Olivier Langella[4]; Véronique Monnet[2]; Catherine Juste[2]; the ProteoCardis Consortium[1,2,4,5,6,7]; *[1]PAPPSO, Micalis Institute, INRA, AgroParisTech, Université Paris-Saclay, Jouy en Josas, France; [2]Micalis Institute, INRA, AgroParisTech, Université Paris-Saclay, Jouy en Josas, France; [3]US1367 MetaGenoPolis, INRA, Jouy en Josas, France; [4]PAPPSO, GQE Le Moulon, INRA, Univ. Paris-Sud, CNRS, AgroParisTech, Universite Paris-Saclay, Gif Sur Yvette, France; [5]Institut National de la Recherche Agronomique, MaIAGE, INRA, Université, Paris-Saclay, Jouy en Josas, France; [6]Institute of Cardiometabolism and Nutrition, ICAN, Assistance Publique Hôpitaux de Paris and Inserm/Sorbonne University team NutriOmics,, Pitié-Salpêtrière Hospital,, Paris, France; [7]Laboratoire de Spectrométrie de Masse BioOrganique, Université de Strasbourg, CNRS, IPHC, UMR 7178, Strasbourg, France*

TP 097 **Liquid-Chromatography coupled to Tandem Mass Spectrometry for 28 Bile Acids Profiling in Serum or Liver Samples**; Yoshihiro Izumi[1]; Mikael Levi[2]; Jun Watanabe[2]; Takeshi Bamba[1]; *[1]National University Corporation Kyushu University, Research Center for Transomics Medecine, Fukuoka, Japan; [2]Shimadzu Corporation, Kyoto, Japan*

TP 098 **Characterization of Patient-Derived Colorectal Cancer Cells Using the Proteome and Phosphoproteome Information**; Ryohei Narumi[1]; Keiko Kasahara[1]; Bo Gong[2]; Yuki Shimizu[2]; Ryohei Katayama[2]; Satoshi Nagayama[2]; Jun Adachi[1]; Takeshi Tomonaga[1]; *[1]NIBIOHN, Ibaraki-city, Japan; [2]JFCR, Koto-ku, Japan*

TP 099 **Plasma Proteome Profiling Discovers Novel Proteins Associated with Non-Alcoholic Fatty Liver Disease**; Lili Niu[1,2]; Rajat Gupta[1]; Philipp E. Geyer[1,2]; Nicolai J. Wewer Albrechtsen[1,2]; Lise L. Gluud[3]; Alberto Santos[1]; Sophia Doll[1,2]; Jens J. Holst[3]; Filip K. Knop[3]; Tina Vilsbøll[3]; Anders Junker[3]; Stephan Sachs[4]; Kerstin Stemmer[4]; Timo D. Müller[4]; Matthias H. Tschöp[4]; Susanna M. Hofmann[5]; Matthias Mann[1,2]; *[1]The Novo Nordisk Foundation center for Protein Research, Copenhagen, Denmark; [2]Max Planck Institute of Biochemistry, Martinsried, Germany; [3]Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark; [4]Helmholtz Diabetes Center at Helmholtz Centre Munich & Division of Metabolic Diseases, munich, Germany; [5]Helmholtz Diabetes Center at Helmholtz Zentrum München, Munich, Germany*

CLINICAL ANALYSIS II
100-123

TP 100 **A LC-MS Method for the Measurement of about 250 Compounds of Interest in Toxicology with a Fully-Automated Sample Preparation**; Tiphaine Robin[1]; Alan Barnes[2]; Neil Loftus[2]; Sylvain Dulaurent[1]; Pierre Marquet[1]; Souleiman El Balkhi[1]; Franck Saint-Marcoux[1]; *[1]CHU Limoges, Limoges, France; [2]Shimadzu Corporation, Manchester, United Kingdom*

TP 101 **Clinical Diagnosis of Congenital Disorders of Glycosylation (CDGs) by Flow Injection Analysis Electrospray Ionization Time-of-Flight Mass Spectrometry (FIA-ESI-TOF-MS)**; Caroline M. Watson[1]; Patricia L. Hall[1]; S. Caleb Jerris[1]; *[1]EGL Genetics, Tucker, GA*

TP 102 **Transition Ratios for the Product-Ion-Poor: Activation Energy Modulation in the Absence of Distinct Neutral Losses**; Brian Rappold; *LabCorp, Raleigh, NC*

TP 103 **Induced In-Source Fragmentation for the Quantitation of Inulin by ESI-MS/MS to Assess Renal Function**; Oscar Ekpenyong[1]; Ken Lin[1]; Lufei Hu[1]; Maribel Beaumont[1]; *[1]Merck & Co., Inc., South San Francisco, CA*

TP 104 **Clinical Diagnostics of Lysosomal Storage Diseases in DBS Using New Substrates by MRM-MS**; Brindusa Alina Petre[1,2,3]; Laura Ion[1,2]; Cristina Dimitriu[4]; Stefan Maeser[2]; Wolfgang Kleinekofort[2]; Cosmin Bulei[1]; Michael Przybylski[2]; *[1]Al. I. Cuza University of Iasi, Iasi, Romania; [2]Steinbeis Centre Biopolymer Analysis and Biomedical Mass Spectrometry, Ruesselsheim, Germany; [3]TRANSCEND - Regional Institute of Oncology, Iasi, Romania; [4]Grigore T. Popa University of Medicine and Pharmacy, Department of Biochemistry, Iasi, Romania*

TP 105 **A UHPLC-MS/MS Method for the Separation and Low-Level Determination of Catecholamines and Metanephrines in Urine Using a Novel C18-Based Column**; Geoffrey Faden[1]; Alan P Mckeown[2]; *[1]MACMOD Analytical Inc., Chadds Ford, PA; [2]Advanced Chromatography Technologies Ltd, Aberdeen, United Kingdom*

TP 106 **Irradiative Sterilization Effects on Clinical Specimens Prior to Mass Spectrometric Analyses**; Samantha L Isenberg[1]; Melissa D Carter[2]; Jonathan L Moon[2]; Sarah Laughlin[2]; Marla Petway[2]; Mike A Mojica[2]; Cody I Sheppard[2]; Alexis K Gursky[2]; Dennis A Bagarozzi Jr.[2]; James L Pirkle[2]; Rudolph C. Johnson[2]; *[1]Centers for Disease Control and Prevention, Atlanta, GA; [2]Centers for Disease Control and Prevention, Atlanta, Georgia*

TP 107 **Analysis of Drugs in Whole Blood by PaperSpray-FAIMS-MS/MS**; Rae Ana Snyder[1]; Cornelia Boeser[1]; Neloni Wijeratne[1]; Mary L. Blackburn[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

TP 108 **Rapid, Direct and Quantitative Urine Analysis for Common and Emerging Drugs of Abuse by Paper Spray Mass Spectrometry (PS-MS)**; Scott A. Borden[1,2]; Jan Palaty[3]; Erik T. Krogh[1,2]; Christopher G. Gill[1,2,4,5]; *[1]Appl. Env. Res. Labs. (AERL), Vancouver Island University, Chemistry Department, Nanaimo, BC; [2]University of Victoria, Chemistry Department, Victoria, BC; [3]Lifelabs Medical Laboratories, Burnaby, BC; [4]Simon Fraser University, Chemistry Department, Burnaby, BC; [5]University of Washington, DEOHS, Seattle, WA*

TP 109 **Evaluation and Quantitation of Nineteen Bile Acids in Human Plasma by LC-MS Analyses**; Hongyi Cai[1]; Peter J. Walter[1]; Mayte Gonzalez[1,2]; *[1]NIH, Bethesda, MD; [2]Schreiner University, Kerrville, TX*

TP 110 **Desorption Electrospray Ionization Mass Spectrometry as a Tool for Diagnosis of Thyroid Nodules from Fine Needle Aspiration Biopsies**; Rachel J DeHoog[1]; Jialing Zhang[1]; Elizabeth Alore[2]; John Lin[1]; Spencer Woody[1]; Wendong Yu[2]; Christopher Almendariz[1]; Monica Lin[1]; Christopher Pirko[2]; Anton F Engelsman[3]; Stan B Sidhu[3];

Robert Tibshirani[4]; James Suliburk[2]; Livia S Eberlin[1]; *[1]University of Texas at Austin, Austin, TX; [2]Baylor College of Medicine, Houston, TX; [3]University of Sydney, Sydney, Australia; [4]Stanford University, Stanford, CA*

TP 111 **High Throughput Analysis of Serum for PFAS Compounds by Reversed Phase High Performance Liquid Chromatography Tandem Mass Spectrometry**; Jessica M. Morrison[1]; Michael C. Stagliano[1]; Timothy A. Karrer[1]; Matthew J. Geiger[1]; *[1]MI Dept of Health & Human Services, Lansing, MI*

TP 112 **Molecular Detection of Pancreatic Ductal Adenocarcinoma in Pancreatic and Bile Duct Tissues Using the MasSpec Pen**; Mary King[1]; Jialing Zhang[1]; John Q. Lin[1]; Sadhna Dhingra[2]; Wendong Yu[2]; George van Buren[2]; William E. Fisher[3]; James Suliburk[3]; Livia S Eberlin[1]; *[1]University of Texas at Austin, Department of Chemistry, Austin, TX; [2]Department of Pathology and Immunology, Baylor College of Medicine, Houston, TX; [3]Department of Surgery, Baylor College of Medicine, Houston, TX*

TP 113 **Application of Mass-Spectrometry for Thalassemia Screening**; Weining Zhao[1]; Rong Wang[1]; Liang lin[1]; *[1]BGI-Shenzhen, Beishan Industrial Zone 11th Building, Yantian District, Shenzhen City, China*

TP 114 **Library Build and Patient Assays from 4- & 15-micron Kidney Biopsies**; Wouter Knol[1]; Petra Jansen[1]; Jesper Kers[1, 2]; Garry Corthals[1]; *[1]University of Amsterdam, Amsterdam, Netherlands; [2]Amsterdam UMC, Amsterdam, Netherlands*

TP 115 **Revealing Proteomic Subgroups with Clinical Classification and Prognostic Prediction in Pancreatic Ductal Adenocarcinoma Using MRM-MS**; Minsoo Son[1]; Yoseop Kim[1]; Jinyoung Jang[2]; Youngsoo Kim[1]; *[1]Department of Biomedical Engineering, Seoul National University College of Medicine, Jongro-gu, South Korea; [2]Department of surgery, Seoul National University College of Medicine, Jongro-gu, South Korea*

TP 116 **Liberate, Equilibrate and Automate; Immunosuppressant Analysis in Whole Blood**; Stacy Dee[1]; Julia Hannon[1]; Matthew Crawford[1]; Russell Grant[1]; *[1]LabCorp, Burlington, NC*

TP 117 **An integrated Pipeline from SWATH Acquisition to MRMHR Workflow Facilitates Identification and Verification of Prostate Diagnostic Markers**; Rui Sun[1]; Christie Hunter[2]; Chen Chen[3]; Xue Cai[1]; Qiushi Zhang[1]; Bo Wang[4]; Xiaoyan Yu[5]; Huanhuan Gao[1]; Xiaodong Teng[4]; Lirong Chen[5]; Ruedi Aebersold[6]; Yi Zhu[1]; Tiannan Guo[1]; *[1]School of Life Sciences, Westlake University, Hangzhou, China; [2]Sciex, Redwood City, CA; [3]Sciex, Shanghai, China; [4]Department of Pathology, The First Affiliated Hospital of College of Medicine, Zhejiang University, Hangzhou, China; [5]Department of Pathology, The Second Affiliated Hospital, Zhejiang University School of Medicine, Hangzhou, China; [6]Department of Biology, Institute of Molecular Systems Biology, ETH Zurich, Switzerland, Switzerland*

TP 118 **Bioanalytical Method for Quantification of Polymyxin B1, Polymyxin B2, Polymyxin B3 and Isoleucine-Polymyxin B1 in Human Plasma**; Peiling Hou[1]; Shu Qing Chan*[2]; Jie Xing[3]; *[1]Application Development & Support Centre, Shimadzu (Asia Pacific) Pte Ltd., 79 Science Park Drive #02-01/08, Singapore; [2]School of Chemical and Life Sciences, Singapore Polytechnic, 500 Dover Road, Singapore; [3]Application Development & Support Centre, Shimadzu (Asia Pacific) Pte Ltd, 79 Science Park Drive #02-01/08, Singapore*

TP 119 **Quantitation of Insulin-Like Growth Factor-1 in Serum by MRM-LC-MS/MS**; Yihan Li[1]; Ji Jiang[1]; Lei Xiong[1]; Xiang He[1]; *[1]SCIEX, Redwood Shores, CA*

TP 120 **A New Approach without Renal Biopsy for Ankylosing Spondylitis with IgA Nephropathy Diagnosis by Glycan Analysis**; Hui-Ling Chiang[1, 2]; Pai-Chi Syue[1]; Ching-Yi Lien[1]; Ning-Sheng Lai[2]; Kuo-Lung Ku[1]; *[1]National Chiayi University, Chiayi City, Taiwan; [2]Dalin Buddhist Tzu Chi Hospital, Dalin Town, Taiwan*

TP 121 **Measurement of Free Drug Concentration from Biological Tissue by Solid-phase Microextraction: In-Silico and Experimental Study**; Mohammad Maududul Hug[1]; Marcos Tascon[2]; Emir Nazdrajić[1]; Anna Roszkowska[3]; Janusz Pawliszyn[1]; *[1]University of Waterloo, Waterloo, ON; [2]Instituto de Investigación e Ingeniería Ambiental (3iA), Universidad Nacional de San Martín (UNSAM), Buenos Aires, Argentina; [3]Department of Pharmaceutical Chemistry, Medical Uni-versity of Gdańsk,, Gdańsk, Poland*

TP 122 **Identification of Circulating Fragments of Human Pancreatic Polypeptide Following Antibody Capture and Liquid Chromatography High Resolution Accurate Mass-Tandem Mass Spectrometry**; Anthony Maus[1]; Robert Taylor[1]; Ravinder Singh[1]; Stefan Grebe[1]; *[1]Mayo Clinic, Rochester, MN*

TP 123 **High-Sensitivity Analysis of Aldosterone in Low-Volume Serum Samples Using Micro-Flow LC-MS/MS for Clinical Research**; Mikael Levi[1]; Jun Watanabe[2]; *[1]SHIMADZU Corporation, Kyoto, Japan; [2]Shimadzu Corpration, Kyoto, Japan*

DISEASE BIOMARKERS I
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TP 124 **Immunopeptide Characterization Enhanced with Positive and Negative Mode 193 nm UVPD**; Eleanor C Watts[1]; Melanie J Patterson[2]; Gregory K Potts[2]; Alayna George Thompson[2]; Damien B Ready[2]; Jennifer S Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX; [2]AbbVie Inc., North Chicago, IL*

TP 125 **Analysis of Ischemic Brain Proteome in Mice in Identifying Clusterin as a Serum Biomarker for Severity of Acute Ischemic Stroke**; Zezong Gu[1]; Hailong Song[1]; Chenghan Wu[2]; Jiankun Cui[1]; *[1]University of Missouri School of Medicine Patholog, Columbia, MO; [2]The Second Affiliated Clinical College, Fujian University of Traditional Chinese Medicine, Fuzhou, China*

TP 126 **Urine from the Patients with Vesicoureteral Reflux Reveals Changes in Host and Bacterial Metabolism after Urinary Tract Infection**; Dijana Vitko[1]; Kohei Hasegawa[2]; Joseph W. McQuaid[3]; Kylie H. Davis[1]; Maggie R. Leary[1]; Shannon E. DiMartino[1]; Jonathan M. Mansbach[1]; Richard S. Lee[1]; *[1]Boston Children's Hospital, Boston; [2]Massachusetts General Hospital, Boston, Massachusetts; [3]University of Massachusetts Medical School, Worcester, MA*

TP 127 **Ganglioside Biomarker Discovery and Characterization in Neuro Developmental Diseases by High Resolution Multistage Mass Spectrometry**; Mirela Sarbu[1]; Raluca Ica[1]; Cristian VA Munteanu[2]; Alina Petrut[1]; Alina D Zamfir[1]; *[1]National Institute for Research and Development in Electrochemistry and Condensed Matter, Timisoara, Romania; [2]Institute of Biochemistry of the Romanian Academy, Bucharest, Romania*

TP 128 **Novel Stationary Phase Aids in the Fight Against Cardiovascular Disease**; Robert Puryear; *Imtakt USA, Portland, OR*

TP 129 **Identification, Validation, and Quantitation of a Clinically Relevant PSA Variant in Post-DRE Urines by Targeted Mass Spectrometry**; Joseph J. Otto[1]; Vanessa L. Correll[1]; Hampus Engstroem[1]; Brian P. Main[1]; Brandi Weaver[2]; Teresa Johnson-Pais[2]; Li Fang Yang[1, 3]; Paul C. Boutros[4]; Thomas Kislinger[5]; Robin J. Leach[2, 6]; O. John Semmes[1, 3]; Julius O. Nyalwidhe[1, 3]; *[1]Leroy T. Canoles Jr. Cancer Research Center, Eastern Virginia Medical School, Norfolk, VA; [2]Department of Urology, The University of Texas Health San Antonio, San Antonio, TX; [3]Department of Microbiology and Molecular Cell Biology, Eastern Virginia Medical School, Norfolk, VA; [4]University of California Los Angeles,*



Los Angeles, CA; [5]University of Toronto, Toronto, ON; [6]Department of Cell Systems and Anatomy, The University of Texas Health San Antonio, San Antonio, TX

TP 130 **Proteomic Insights into the Molecular Mechanisms of Breast Cancer Metastasis**; Shreya Ahuja[1]; Iulia M. Lazar[1]; *[1]Virginia Tech, Blacksburg, VA*

TP 131 **Proteomic Analysis of the HBP-Induced TIFA Interactome**; Tong-You Wade Wei[1]; Chi-Chi Chou[1]; Wan-Jyun Lin[1]; Pei-Yu Wu[1]; Ming-Daw Tsai[1]; *[1]Academia Sinica, Taipei, Taiwan*

TP 132 **Analysis of Metabolome and Lipidome Reveals the Metabolic Changes in Hypothermia Treatment of Cardiac Arrest Patients**; Daniel Contaifer Jr.[1]; Naren Gajenthra Kumar[2]; Joshua Morriss[1]; Dayanjan S Wijesinghe[1]; *[1]Department of Pharmacotherapy and Outcomes Sciences, Virginia Commonwealth University, Richmond, VA; [2]Department of Microbiology and Immunology, Virginia Commonwealth University, Richmond, VA*

TP 133 **Investigation of AD and MCI Associated Changes in Blood Plasma Proteome by High Resolution Mass Spectrometry**; Natalia V. Zakharova[1,2]; Anna Bugrova[1]; Maria Indeykina[1,2]; Alexander Brzhozovskiy[3,4]; Yana B. Fedorova[5]; Svetlana I. Gavrilova[5]; Igor Popov[2]; Alexey Kononikhin[2,3]; Eugene (evgeny) Nikolaev[4]; *[1]Emanuel Institute for Biochemical Physics, Russian Academy of Sciences, Moscow, Russia; [2]Moscow Institute of Physics and Technology (State University), Dolgoprudny, Russia; [3]V.L. Talrose Institute for Energy Problems of Chemical Physics, Russian Academy of Sciences, Moscow, Russia; [4]Skolkovo institute of science and technology, Moscow Region, Russian Federation; [5]Mental Health Research Center, Russian Academy of Science, Moscow, Russia*

TP 134 **Detection of Anthrax Toxins in Terminal Organ Tissues by Mass Spectrometry**; Maribel Gallegos Candela[1]; Anne E Boyer[1]; Adrian R. Woolfitt[1]; Renato C. Lins[2]; Maria I. Solano[1]; John R. Barr[1]; *[1]Center for Disease Control, Atlanta, GA; [2]Battelle Integrated Science Solutions, Atlanta, GA*

TP 135 **Analysis of Human Skin Wound Healing Process Using 2D-TOF-SIMS**; Anthony Castellanos[1]; Ivan Jozic[2]; Francisco A. Fernandez-Lima[3,4]; *[1]Florida International University, Miami, FL; [2]Dr. Phillip Frost Department of Dermatology & Cutaneous Surgery, University of Miami Miller School of Medicine, Miami, FL; [3]Department of Chemistry and Biochemistry, Florida International University, Miami, FL; [4]Biomolecular Sciences Institute, Florida International University, Miami, FL*

TP 136 **Global Protein Expression Alterations Linked to TDP-43 Dysregulation of Cryptic Exon Expression**; Shivangi Awasthi[1]; Rachel Korn[1]; Robert E. Drolet[1]; Jonathan P. Ling[2]; Philip C. Wong[2]; Sophie P. Batteur[1]; Sean M. Smith[1]; Nathan G. Hatcher[1]; *[1]Merck & Co. Inc., Kenilworth, New Jersey; [2]Departments of Pathology and Neuroscience, The Johns Hopkins University School of Medicine, Baltimore, MD*

TP 137 **Prediction of ZIKV Infection in Mosquitoes by MS Analysis of RNA Modification Biomarkers**; Rachel Netzband[1,2]; Will McIntyre[1,2]; Gaston Bonenfant[1,2]; Sean Bialosuknia[3]; Alexander Ciota[3]; Cara T. Pager[1,2]; Daniele Fabris[1,2]; *[1]University at Albany, Albany, NY; [2]The RNA Institute, University at Albany, Albany, NY; [3]Wadsworth Center, Department of Health, Albany, NY*

TP 138 **Quantification of Full Length and Activated Anthrax Protective Antigen by Immunocapture and Isotope Dilution Mass Spectrometry**; Maria I. Solano[1]; Adrian R. Woolfitt[1]; Anne E. Boyer[1]; Renato C. Lins[2]; Maribel Gallegos-Candela[1]; Hercules Moura[1]; Carrie L. Pierce[1]; John R. Barr[1]; *[1]Centers for Disease Control and Prevention, Atlanta, GA; [2]Battelle Memorial Institute at the Centers for Disease Control and Prevention, Atlanta, GA*

TP 139 **Integrating Spectral Library Search and Database Search to Improve Endogenous Peptide Identification**; Lei Xin[1]; Xin Chen[1]; Zhewei Liang[1]; Wenju Zhang[1]; Baozhen Shan[1]; *[1]Bioinformatics Solutions Inc., Waterloo, ON*

TP 140 **Is NAP Treatment a Solution for Neuroprotection in ADNP Mutation Syndrome?**; Ming-Hui Yang[1]; Yi-Chia Lee[2]; Hsin-Yi Wu[3]; Ko-Chin Chen[4]; Yi-Ming Arthur Chen[5]; Yu-Chang Tyan[2]; *[1]National Health Research Institutes, Zhunan, Taiwan; [2]Kaohsiung Medical University, Kaohsiung, Taiwan; [3]National Taiwan University, Taipei, Taiwan; [4]Changhua Christian Hospital, Changhua, Taiwan; [5]Taipei Medical University, Taipei, Taiwan*

TP 141 **Proteomic Profiling in Hematopoietic Tissues of Jak2 Conditional Knock-Out Mice**; Jin Koh[1]; Sung Park[1]; Mi-Jeong Yoo[1]; Sixue Chen[1]; Peter Sayeski[1]; *[1]University of Florida, Gainesville, FL*

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TP 142 **Novel Fractionation Techniques Applied to Oil-Contaminated Residues Characterized by FT-ICR Mass Spectrometry Reveal the Complexity of Ox Transformation Products**; Cameron C. Davis[1]; Amy Mckenna M. Mckenna[2]; Huan Chen[2]; Ryan P. Rodgers[2,3]; Sydney Niles[2,3]; Martha Chacón-Patiño[2]; Qianxin Lin[4]; Aixin Hou[5]; *[1]National High Magnetic Field Laboratory, Tallahassee, FL; [2]National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; [3]Department of Chemistry and Biochemistry, Florida State University, Tallahassee, FL; [4]Department of Oceanography and Coastal Sciences, College of the Coast and Environment, Louisiana State University, Baton Rouge, LA; [5]Department of Environmental Sciences, College of the Coast and Environment, Louisiana State University, Baton Rouge, LA*

TP 143 **Fourier Transform Ion Cyclotron Resonance Mass Spectrometry Reveals the Role of Heteroatoms in Asphaltene Chemistry**; Martha Liliana Chacón-Patiño[1]; Donald F. Smith[1]; Sydney F Niles[1]; Jonathan C. Putman[1]; Amy M. McKenna[1]; Yuri E. Corilo[1]; Christopher L. Hendrickson[1]; Alan G. Marshall[1]; Ryan P. Rodgers[1]; *[1]National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL*

TP 144 **UPLC-MS/MS Determination of Hexahydro-1,3,5-tris(2-hydroxyethyl)-s-triazine and its Reaction Products in Extra Heavy Crude Oil**; Lun-yi Zang[1]; Martin Harper[2,3]; *[1]CDC/NIOSH/HELD, Morgantown, WV; [2]Zefon International, Inc., Ocala, FL; [3]Department of Environmental Engineering Sciences, University of Florida, Gainesville, FL*

TP 145 **Application of Molecular Characterization for fluorine Polymers Using Thermal Desorption/Pyrolysis DART-MS**; Chikako Takei[1]; Kenichi Yoshizawa[1]; Derek Gonzales[2]; Sayaka Nakamura[3]; Hiroaki Sato[3]; *[1]BioChromato, Inc., Fujisawa, Japan; [2]BioChromato USA, San Diego, California; [3]National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan*

TP 146 **Speciation of Asphaltenes Using Mass-Deficient Tagging Mass Spectrometry and Metal-Reduced Nuclear Magnetic Resonance Spectroscopy**; Ian Anthony[1]; Michael T. Spiegel[1]; Annie Arvidson[1]; Shubhneet Warar[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX*

TP 147 **Inductively Coupled Plasma-Mass Spectrometry Characterization of Asphaltene Metals Pre- and Post-Cleanup for Enhanced Nuclear Magnetic Resonance Spectroscopy Results**; Annie E. Arvidson[1]; Ian G. M. Anthony[1]; Michael T. Spiegel[1]; Shubhneet Warar[1]; Patrick J. Farmer[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX*

TP 148 **Structural Comparison of Nickel and Vanadyl Porphyrins from Natural Seeps and the 1.1-Billion-Year-Old Shale Oil**; Huan Chen[1]; Martha L. Chacón-Patiño[1];

Chad Weisbrod[1]; Gregory T. Blakney[1]; Jochen Brocks[2]; Nur Guneli[2]; Nao Ohkouchi[3]; Chris J. Boreham[4]; Jérémie Beghine[5]; David Valentine[6]; Matthias Kellermann[5]; Ryan P. Rodgers[1]; Amy McKenna[1]; *[1]National High Magnetic Field Laboratory, Tallahassee, FL; [2]Australian National University, Canberra, Australia; [3]Japan Agency for Marine–Earth Science and Technology, Yokosuka, Japan; [4]Geoscience Australia, Symonston, Australia; [5]University of Liège, Liège, Belgium; [6]University of California, Santa Barbara, CA*

TP 149 **Increasing Analytical Separation of Polycyclic Aromatic Hydrocarbons from Crude Oils Using GC-TIMS-MS**; Clement Ajibade Olanrewaju[1]; Cesar E. Ramirez[2]; Francisco Fernandez-Lima Fernandez Lima[3]; *[1]Department of Chemistry and Biochemistry, Florida International University, Miami, FL; [2]Advance Mass Spectrometry Facility, Department of Chemistry and Biochemistry, Florida International University. Miami Florida, Miami, FL; [3]Department of Chemistry and Biochemistry, Florida International University, Mimai, FL*

TP 150 **CID Fragmentation Studies of Asphaltenes at Different Precipitation Times Using Magnetic Resonance Mass Spectrometry (MRMS)**; Matthias Witt[1]; Michael L. Easterling[2]; Estrella Rogel[3]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Bruker Daltonics Inc., Billerica, MA; [3]Chevron, Richmond, CA*

TP 151 **Analysis of Jet Fuel Thermal Oxidative Deposits by Pyrolysis Gas Chromatography/Mass Spectrometry**; Krege Matthew Christison[1, 2]; Michael Browne[2]; Tommy Nguyen[2]; O. David Sparkman[2]; *[1]Chevron, Richmond, CA; [2]University of the Pacific, Stockton*

TP 152 **Evaluation of Time Effects on Precipitated Asphaltene Characteristics Using APPI and LDI coupled to Magnetic Resonance Mass Spectrometry (MRMS)**; Estrella Rogel[1]; Matthias Witt[2]; Michael Moir[1]; *[1]Chevron, Richmond, CA; [2]Bruker Daltonik GmbH, Bremen, Germany*

TP 153 **Electron-Transfer Ionization in MALDI-MS for the Direct Targeted Analysis of Metalloporphyrins in Complex Mixtures**; Juan Ramirez[1]; Cristian Blanco-Tirado[1]; Pierre Giusti[2]; Carlos Afonso[3]; Marianny Y. Combariza[1]; *[1]Universidad Industrial de Santander, Bucaramanga, Colombia; [2]Total Research & Technology Gonfreville, Harfleur, France; [3]University of Rouen, Mont Saint Aignan, France*

TP 154 **New Insights in Crude Oil Using MS, NMR, and EPR**; Michael T. Spiegel[1]; Ian G. M. Anthony[1]; Shubhneet Warar[1]; Annie Arvidson[1]; Anish Sasmal[1]; Touradj Solouki[1]; Patrick J. Farmer[1]; *[1]Baylor University, Waco, TX*

TP 155 **(+/-) ESI FT MS Analysis of Crude Oils from the Volga-Ural Region**; Vlad Lobodin[1]; Dmitrii Mazur[2]; Roman Borisov[3]; *[1]MAXIKAT, INC, Tallahassee, FL; [2]The Department of Chemistry, Moscow State University, Moscow, Russia; [3]A.V. Topchiev Institute of Petrochemical Synthesis, Moscow, Russia*

TP 156 **Fast, Robust, 'Dilute and Shoot' Screening of Adulterated Low Taxation Fuels**; G. John Langley[1, 2]; Julie M. Herniman[1]; James Barker[2, 3]; *[1]University of Southampton, Southampton, United Kingdom; [2]Energy Institute, London, United Kingdom; [3]Innospec Inc., Ellesmere Port, United Kingdom*

TP 157 **Development of Predictive Methods of Sulfur Content in Hydropyrolysis Oil Products by Elemental Sulfur Analysis of Crude Oil Feedstocks**; Kyle L. Wilhelm[1]; Drew Stolpman[2]; Zhao Wang[1]; Bill Hockaday[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX; [2]Baylor Univeristy, Waco, TX*

TP 158 **Hydrocarbons High Mass Profiling of Crude and Commercial Oils Using LDTD-HRMS Technology**; Jonathan Rochon[1]; Pier-Luc Plante[1]; Serge Auger[2]; Jean Lacoursière[2]; Pierre Picard[2]; *[1]Université Laval, Québec, QC; [2]Phytronix Technologies, Inc., Quebec, QC*

TP 159 **Development of Quantitative Isotope Labeling IC-MS/MS method for Phosphonate Scale Inhibitors Analysis**; Lei (Lyla) Cheng[1]; Christopher Durnell[1]; Robert Pultz[1]; Manojkumar Bhandari[1]; Christine Kerr[1]; Emerilis Casado-Rivera[1]; *[1]Nalco Champion, Sugar Land, TX*

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TP 160 **Simultaneous Detection of 12 Microcystins, Nodularin, Cylindrospermopsin, and Anatoxin-a**; Matthew Prescott[1]; Yingbo C. Guo[1]; Ali Haghani[2]; Andrew Eaton[2]; *[1]Metropolitan Water District of Southern California, La Verne, CA; [2]Eurofins Eaton Analytical, 750 Royal Oaks Drive, Monrovia, CA*

TP 161 **Analysis of Drinking Water for Determination of Volatile Organic Components (VOC's) Using Dynamic Headspace Gas Chromatography Mass Spectrometry**; Sanket Anand Chiplunkar[1]; Dheeraj Handique[1]; Prashant Hase[1]; Durvesh Sawant[1]; Nitish Suryawanshi[1]; Aseem Wagle[1]; Pratap Rasam[1]; Jitendra Kelkar[1]; Ajit Datar[1]; Satyendra Thakur[2]; Sunil Singh[2]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India; [2]Shimadzu Analytical (India) Pvt. Ltd., New Delhi, India*

TP 162 **Trace Analysis of PFAS in Environmental and Serum Samples by Micro-SPE**; Andrew Minett[1]; Mohammad Talebi[2]; Thomas Lockwood[3]; *[1]EPREP, Mulgrave, Australia; [2]Envirolab, Sydney, Australia; [3]University of Technology Sydney, Sydney, Australia*

TP 163 **Structural Elucidation of the Direct Photolysis Transformation Products of a Halogenated Estrogen**; Keeton T. Nance[1]; Carolyn P. Hutchinson[1]; David R. Griffith[1]; *[1]Willamette University, Salem, OR*

TP 164 **Developing an Untargeted High-resolution Mass Spectrometry Method for the Detection and Identification of Glucuronide Biotransformation Products in Environmentally Exposed Fish**; Marina Evich[1]; Jonathan Mosley[2]; Ioanna Ntai[3]; Drew Ekman[2]; Timothy Collette[2]; *[1]ORISE Fellow, US EPA, Athens, GA; [2]US EPA, Athens, GA; [3]ThermoFisher Scientific, San Jose, CA*

TP 165 **A Novel Mass Spectrometric Method to Measure Siloxanes**; Eleanor Browne[1]; Mitchell Alton[1]; *[1]University of Colorado Boulder, Boulder, CO*

TP 166 **Improved Non-Target Screening Based Identification of Organic Micropollutants in Water Samples**; Andrea Mizzi Brunner[1]; Seema Sharma[2]; Christian Panse[3]; Romain Huguet[2]; Dennis Vughs[1]; Vlad Zabrouskov[2]; Annemieke Kolkman[1]; *[1]KWR Watercycle Research Institute, Nieuwegein, Netherlands; [2]Thermo Fisher Scientific, San Jose, Ca, 95134; [3]Functional Genomics Center Zurich, Zurich, Switzerland*

TP 167 **You Can Only See What You Can Ionize: A Comparison of Ionization Techniques for Dissolved Organic Matter Mass Spectrometric Characterization**; Juliana R Laszakovits[1]; Allison A MacKay[1]; *[1]The Ohio State University, Columbus, OH*

TP 168 **Toxin Identification and Correlation to Biological Endpoints Using Multivariate Data Analysis: An LC-HRMS Top-Down Approach to Discerning Differential Toxicological Responses**; Raegyn B. Taylor[1]; Jonathan M. Bobbitt[1]; Bridgett N. Hill[1]; Amanda S. Hering[1]; Bryan W. Brooks[1]; Kevin Chambliss[1]; *[1]Baylor University, Waco, TX*

TP 169 **Gestational Exposure to Benzotraizoles and Benzothiazoles in Relation to Birth Weight: A Repeated Measures Study**; Yanqiu Zhou[1]; Zongwei Cai[2]; *[1]Hong Kong Baptist University, Hong Kong, Hong Kong; [2]Hong Kong Baptist University, Hong Kong, China*

TP 170 **A Direct Inject Approach for Analysis of Legacy and Emerging Perfluoroalkyl Substances in Environmental Water and Soil Samples**; Kari Organtini[1]; Kenneth Rosnack[1]; Doug Stevens[1]; Aurelie Marcotte[1]; *[1]Waters Corporation, Milford, MA*

TP 171 **Ultrafast Trace Quantitation of PFAS in Drinking and Environmental Waters Using an Automated Sample Preparation and LC-MS/MS System**; Nigel Grieves[1]; David Humberstone[1]; Cindy Si Ni Lee[2]; Atsuhiko Toyama[2]; *[1]Shimadzu Scientific Instruments Oceania, Sydney, Australia; [2]Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore*

TP 172 **Drinking Water Safety and Sustainability: Using Mass Spectrometry to Identify Chemical Drivers of Toxicity**; Joshua M. Allen[1]; Michael J. Plewa[2]; Jia Ai[3]; Carrie Guo[3]; Amy A. Cuthbertson[1]; Hannah K. Liberatore[1]; Tiffany Lee[3]; Raha Shirkhani[3]; Stuart W. Krasner[3]; Susan D. Richardson[1]; *[1]University of South Carolina, Columbia, SC; [2]University of Illinois at Urbana Champaign, Urbana, IL; [3]Metropolitan Water District of Southern California, La Verne, CA*

TP 173 **Fast Semi-Automated Extractable Petroleum Hydrocarbons Fractionation and Cleanup**; Tom Hall[1]; Ruud Addink[1]; *[1]Fluid Management Systems, Watertown, MA*

TP 174 **Understanding the Structural Complexity of Dissolved Organic Matter: Isomeric Diversity**; Dennys Leyva[1]; Lilian V. Tose[1]; Jacob Porter[1]; Jeremy Wolff[2]; Rudolf Jaffé[3]; Francisco A. Fernandez-Lima[1,4]; *[1]Department of Chemistry and Biochemistry, Florida International University, Miami, FL; [2]Bruker Daltonics Inc., Billerica, MA; [3]Southeast Environmental Research Center, Florida International University,, Miami, FL; [4]Biomolecular Sciences Institute, Florida International University, Miami, FL*

TP 175 **Detection and Quantification of Nine Haloacetic Acids with Ion Chromatography Mass Spectrometry**; Phuc Nguyen[1]; David Clases[1]; David Bishop[1]; Philip Doble[1]; *[1]University of Technology Sydney, Sydney, Australia*

TP 176 **Chemicals in Textiles: A Source of Environmental Pollution and Human Exposure?**; Francesco Iadaresta[1]; Carlo Crescenzi[2]; Conny Ostman[3]; *[1]stockholm university, stockholm, Sweden; [2]University of Salerno, Salerno, Italy; [3]Stockholm University, Stockholm, Sweden*

TP 177 **Integrated Use of QTOF and Q-Exactive Orbitrap Mass Spectrometry for Suspect and Non-Target Screening of Emerging Pollutants in Wastewater**; Hailemariam A Assress[1]; Hlengilizwe H. Nyoni[1]; Bhekie B. Mamba[1]; Titus TAM Msagati[1]; *[1]University Of South Africa(UNISA), Johannesburg, South Africa*

TP 178 **High-Throughput Determination of Seventeen Cyanotoxins and Suspect Screening of Other Cyanopeptides by SPE-UHPLC-HRMS in Canadian Lakes**; Audrey Roy-Lachapelle[1]; Sung Vo Duy[2]; Dinh Quoc Tuc[2]; Gabriel Munoz[2]; Sébastien Sauvé[2]; Christian Gagnon[1]; *[1]Environment and Climate Change Canada, Montréal, QC; [2]University of Montreal, Montreal, QC*

TP 179 **Arsenic and Thioarsenic Speciation Using Ion Chromatography Mass Spectrometry**; Tisa Campbell[1]; Jianye Zhang[1]; *[1]Voorhees College, Denmark, SC*

TP 180 **Direct Photolysis Transformation Products from Brominated Estrogens in Treated Wastewater Effluent**; Carolyn P. Hutchinson[1]; Keeton T. Nance[1]; David R. Griffith[1]; *[1]Willamette University, Salem, OR*

TP 181 **Photolysis of Emerging Contaminants Absorbed on Plastic Debris in an Aqueous Environment**; Xiolmara Martinez[1]; Daryl Giblin[2]; Angeline Alag[1]; Kathryn Renyer[1]; Michael L Gross[2]; M. Paul Chiarelli[1]; *[1]Loyola University, Chicago, IL; [2]Washington University, St. Louis, MO*

TP 182 **High Throughput Analysis of Deer Tissue for Perfluorinated Compounds by Reversed Phase High Performance Liquid Chromatography Tandem Mass Spectrometry**; Michael C. Stagliano[1]; Jessica M. Morrison[1]; Timothy A. Karrer[1]; Matthew J. Geiger[1]; *[1]MI Dept of Health & Human Services, Lansing, MI*

TP 183 **A New Method for a Systematic Analysis of Siderophores in Soils**; Vineeta Rai[1]; Oliver Baars[1]; *[1]North Carolina State University, Raleigh, NC*

TP 184 **A Single Analytical Method for the Determination of Legacy and Emerging Per- and Poly Fluoroalkyl Substances (PFAS) in Aqueous Matrices**; Timothy Coggan[1]; Tarun Anumol[2]; Bradley Clarke[1]; *[1]RMIT University, Melbourne, Australia; [2]Agilent Technologies, Wilmington, DE*

TP 185 **Moving Beyond Monitoring Legacy Per and Polyfluoroalkyl Substances (PFAS): Screening Strategies for the Growing List**; James S Pyke[1]; Tarun Anumol[2]; Jerry A. Zweigenbaum[2]; *[1]Agilent Technologies, Inc., Santa Clara, CA; [2]Agilent Technologies, Inc., Wilmington, DE*

TP 186 **Identification and Quantification of Microcystins in Western Lake Erie during 2016 and 2017 Harmful Algal Blooms**; Dilrukshika S W Palagama[1]; David Baliu-Rodriguez[1]; Brenda K Snyder[1]; Jennifer A Thornburg[1]; Thomas B Bridgeman[1]; Dragan Isailovic[1]; *[1]University of Toledo, Toledo, OH*

TP 187 **Fast Semivolatiles Method by GC/MS/MS that Meets EPA 8720D/E Requirements**; Melissa Churley[1]; Bruce Quimby[2]; Anastasia Andrianova[2]; *[1]Agilent, Santa Clara, CA; [2]Agilent, Wilmington, DE*

TP 188 **Determination of 8 Nitrosamines in Water by Liquid Chromatography Coupled to Tandem Mass Spectrometry**; Wei Du[1]; Xiaorong Ran[1]; *[1]Agilent Technologies(China) Co. Ltd., Beijing, China*

TP 189 **Automated Liquid-Liquid Extraction for Environmental Analysis**; Masoomeh Tehranirokh[1,2]; Marcel Van de Bronk[2]; Andrew Gooley[1,2]; Peter Smith[3]; Zhengshan Dai[3]; Kyle Bachus[2]; Simon Mills[4]; Robert Shellie[5]; *[1]ARC Training Centre for Portable Analytical Separation Technologies (ASTech), Hobart, Australia; [2]Trajan Scientific and Medical, Ringwood, Australia; [3]Trajan Scientific and Medical, Morrisville, NC; [4]Envirolab, Sydney, Australia; [5]Centre for Advanced Sensory Science (CASS), School of Exercise and Nutrition Sciences, Deakin University, Melbourne, Australia*

TP 190 **Differential Expression of Inflammatory Proteins in New Male and Female Swine Confinement Workers**; Brooke Thompson[1]; Paulos Chumala[1]; David Schneberger[1]; Shelley Kirychuk[1]; George S. Katselis[1]; *[1]University of Saskatchewan, Saskatoon, SK*

TP 191 **Methods for Metaproteomic Analysis of the Ocean**; Matthew McIlvin[1]; Mak Saito[2]; *[1]Woods Hole Oceanographic Inst., Woods Hole, MA; [2]Woods Hole Oceanographic Institution, Woods Hole, MA*

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TP 192 **Quantitation and Localization of Endocrine Disruptor Compounds Accumulation in Fathead Minnows by Complementary Mass Spectrometry Analyses**; Rachel Davis[1]; Sarah Rizzo[1]; Jackson Hoang[1]; Bobbi J Potter[1]; Kevin R Tucker[1]; *[1]Southern Illinois University Edwardsville, Edwardsville, IL*

TP 193 **Micropollutant Removal during Wastewater Treatment: Evaluation of the Process Effectiveness Using High Resolution Accurate Mass LC-MS/MS**; Madhuri Damaraju[1]; Keerthi Katam[1]; Lokesh Kumar Akula[1]; Prasanth Joseph[2]; Saikat Banerjee[2]; Debraj Bhattacharyya[1]; *[1]Indian institute of Technology, Hyderabad, India; [2]Agilent Technologies, Whitefield, Bengaluru, India*

TP 194 **Quantification of Azithromycin in Sheep Tissue Samples Using LCMSMS**; Chander Mani[1]; T.s. Lohith[2]; Saikat Banerjee[1]; Samir Vyas[1]; S.m. Byregowda[2]; K.

Sripad[2]; [1]*Agilent Technologies, Gurgaon, India;* [2]*Institute of Animal Health and Veterinary Biologicals, Bengaluru, India*

TP 195 **Developing Methods to Assess the Environmental Impact of Pesticides and Pharmaceuticals on Aquatic Fauna Using Targeted and Untargeted HRAM Q-TOF**; Christopher Titman[1]; Thomas H Miller[2]; Keng Tiong Ng[2]; Nicholas R Bury[3,4]; Leon P Barron[2]; Alan Barnes[5]; Neil Loftus[5]; [1]*Shimadzu UK Limited, Milton Keynes, United Kingdom;* [2]*Department of Analytical, Environmental & Forensic Sciences, School of Population Health & Environmental Sciences, Faculty of Life Sciences and Medicine, King's College London, United Kingdom;* [3]*School of Science, Technology and Engineering, University of Suffolk, James Hehir Building, University Avenue, Ipswich, United Kingdom;* [4]*Division of Diabetes and Nutritional Sciences, Faculty of Life Sciences and Medicine, King's College London, Franklin Wilkins Building, United Kingdom;* [5]*Shimadzu Corporation, Manchester, United Kingdom*

TP 196 **An LC-MS/MS Study of the Kinetics of Atrazine Decomposition Catalyzed by Interactions with Soil**; Heather Gamble[1]; Donald S Gamble[2]; Jincun Wu[1]; Mitesh Patel[3]; [1]*PerkinElmer Inc., Woodbridge, ON;* [2]*St. Mary's University, Halifax, NS;* [3]*PerkinElmer Inc., Bolton, ON*

TP 197 **ESS-MAT: A New Approach for Simultaneous Analysis of Organophosphate Pesticides and their Degradation Products On Agricultural Products**; noam Kirshenbaum[1]; Tamara Polubesova[1]; Benny Chefetz[1]; [1]*Department of Soil and Water Sciences The Robert H. Smith Faculty of Agriculture, Food and Environment The Hebrew University of Jerusalem, Rehovot, Israel*

TP 198 **Identification and Quantification of Degradation Products in Amoxicillin and Sertraline Stored Aboard the International Space Station**; Virginia K James[1]; Wendy Cory[1]; [1]*College of Charleston, Charleston, SC*

TP 199 **Combination of Targeted and Non-Targeted Workflows for the Identification of Pollutants in River Water Using a Passive Sampling Method**; Anthony Gravell[1]; Melanie Schumacher[1]; Bob Galvin[2]; Carsten Baessmann[3]; [1]*Natural Resources Wales, Swansea University, Swansea, United Kingdom;* [2]*Bruker UK Ltd., Coventry, United Kingdom;* [3]*Bruker Daltonik GmbH, Bremen, Germany*

TP 200 **Trace determination of Octyl & Nonyl-phenols and Ethoxylates and Bisphenol A Using On-Line SPE and Q Exactive Focus Orbitrap LCMSMS**; Nevillee Llewellyn[1]; James Thomas[2]; Olaf Scheibner[3]; Ed George[4]; [1]*ThermoFisherScientific, Hemel Hempstead, United Kingdom;* [2]*Scottish Environment Protection Agency, Glasgow, United Kingdom;* [3]*Thermo Fisher Scientific (Bremen), Bremen, Germany;* [4]*Thermo Fisher Scientific, San Jose, CA*

TP 201 **Simultaneous Targeted Quantification and Suspect Screening of Environmental Contaminates in Sewage Sludge by High Resolution LC-QTOF**; James S Pyke[1]; Gabrielle Black[2]; Kai Chen[1]; Tarun Anumol[3]; Thomas M Young[2]; [1]*Agilent Technologies, Inc., Santa Clara, CA;* [2]*University of California, Davis, Davis, CA;* [3]*Agilent Technologies, Inc., Wilmington, DE*

TP 202 **Fast Creatinine Determination in Wastewater by Liquid Chromatography-Mass Spectrometry**; Lisa Wanders[1]; Matthew Obusek[1]; [1]*Thomson Instrument Co, Oceanside, CA*

TP 203 **Use of Triple Quadrupole Mass Spectrometry to Characterize Antibiotics in Cow Manure**; Andrea Yarberry[1]; Clifford Rice[1]; Carlton Pointexter[2]; Stephanie Lansing[2]; [1]*United States Department of Agriculture, Beltsville, Maryland;* [2]*University of Maryland, College Park, Maryland*

TP 204 **Estrogen Monitoring in River Waters at Low Part Per Trillion Levels by Online SPE-UHPLC-MS/MS**; Jason Weisenseel[1]; Jamie Foss[1]; Wilhad Reuter[1]; [1]*PerkinElmer, Shelton, CT*

TP 205 **Analysis of Pharmaceuticals and Personal Care Products (PPCPs) in Drinking Water at Low Part Per Trillion Levels by Online SPE-UHPLC-MS/MS**; Jamie Foss[1]; Wilhad Reuter[1]; [1]*PerkinElmer, Shelton, CT*

TP 206 **Reliable Determination of Sulfonamides in Environmental Water Matrices Using UHPLC-MS/MS**; Xiulan Zhang[1]; Chaofei Zhu[1]; Jing Guo[1]; Meiling Lu[2]; Liang Dong[1]; Yeru Huang[1]; [1]*National Center for Environmental Analysis and Measurement, Beijing, China;* [2]*Agilent Technologies (China) Limited, Beijing, China*

TP 207 **Exploring the Physicochemical Properties of Pesticides Using Differential Mobility Spectrometry and Machine Learning-Based Modelling**; J. Larry Campbell[1]; J. C. Yves Le Blanc[1]; Brendon Seale[1,2]; Zack Bowman[3]; Jeff Crouse[3]; Ce Zhou[3]; W. Scott Hopkins[3]; [1]*SCIEX, Concord, ON;* [2]*York University, Toronto, ON;* [3]*University of Waterloo, Waterloo, ON*

TP 208 **Orbitrap Assessment of Targeted and Non-Targeted Pharmaceuticals and Personal Care Products in Wastewater Effluents and their Impact on River Water**; Vimbai Mhuka[1]; simiso Dube[2]; Mathew M Nindi[1]; [1]*UNISA, Florida Park, Roodepoort, South Africa;* [2]*UNISA, Florida Park, Roodepoort, South Africa*

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TP 210 **Application of UPLC-MS/MS for Determination of Synthetic Organic Dyes and their Metabolites**; Angelika Tkaczyk[1]; Kamila Mitrowska[1]; Andrzej Posyniak[1]; [1]*National Veterinary Research Institute (PIWet), Pulawy, Poland*

TP 211 **Ultra-Fast Screening of Glyphosate, Glufosinate and AMPA in Surface Water by LDTD-QqQMS**; Cassandra Guérette[1]; Serge Auger[2]; Pierre Picard[2]; Pedro A. Segura[1]; [1]*Universite de Sherbrooke, Sherbrooke, Quebec;* [2]*Phytronix Technologies, Inc., Quebec, QC*

TP 212 **Analysis of Semi-Volatile Organics in Drinking Water with Semi-Automated Solid Phase Extraction Using EPA Method 525.3**; Rashid Juma[1]; Rudolf Addink[1]; [1]*Toxic Report, Watertown, MA*

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TP 215 **Determination of Polar Pesticides in Grapes Using a Compact Ion Chromatography System Coupled with Tandem Mass Spectrometry**; Beibei Huang[1]; Jeffrey Rohrer[1]; [1]*Thermo Fisher Scientific, Sunnyvale*

TP 216 **Highly Sensitive Direct Analysis of Glyphosate, Glufosinate and AMPA in the Beverages by LC-MS / MS**; Manami Kobayashi[1]; Miho Kawashima[2]; Yusuke Inohana[2]; Nozomi Maeshima[1]; Junichi Masuda[1]; Yoshihiro Hayakawa[2]; [1]*Shimadzu Corporation, Hadano, Japan;* [2]*Shimadzu Corporation, Kyoto, Japan*

TP 217 **Analysis of Benzo[a]pyrene in Tobacco and Related Products by Ultra High-Performance Liquid Chromatography - Tandem Mass Spectrometry**; Xia Geng[1]; Jingcun Wu[2]; Lizhong Yang[3]; Feng Qin[2];

[1]PerkinElmer Management(Shanghai)Co.,Ltd., Shanghai, China; [2]PerkinElmer Inc., Woodbridge, Ontario; [3]Perkinelmer Management (Shanghai) Co., Ltd., Shanghai, China

TP 218 **Quantitation of Heterocyclic Amines in Non-Meat Products and their Cancer Risks as Exposed**; Tzu-Sheng Fang[1]; Wei-Lun Su[1]; Yi-Chen Sun[1]; Hsin-Chang Cheng[1]; *[1]Institute of Food Safety and Health, National Taiwan University, Taipei, Taiwan*

TP 219 **Fatty Acid Composition Analysis for Glycerides in Edible Oils Using Thermal Desorption/Pyrolysis DART-QTOFMS**; Kenichi Yoshizawa[1]; Chikako Takei[1]; Michael Churchill[2]; *[1]BioChromato, Inc., Fujisawa, Japan; [2]BioChromato USA, San Diego, California*

TP 220 **Quantitation of Process-Induced Nitrogen Compounds in Foods Using QuEChERS Coupled with UPLC-MS/MS**; Wei Lun Su[1]; Hsin-Chang Chen[1]; *[1]Institute of Food Safety and Health, National Taiwan University, Taipei, Taiwan*

TP 221 **Determination of Pyrrolizidine Alkaloids in Plant Material Using SFC-MS/MS**; Anja Gruening[1]; Gesa J. Schad[1]; Jan Stenzler[2]; *[1]Shimadzu Europa GmbH, Duisburg, Germany; [2]Shimadzu Deutschland GmbH, Duisburg, Germany*

TP 222 **Distribution of Heterocyclic Amines in Fried and Braised Plant Protein Foods**; Kai-Chieh Yang[1]; Yi-Chen Sun[1]; Wei Lun Su[1]; Hsin-Chang Chen[1]; *[1]Institute of Food Safety and Health, National Taiwan University, Taipei, Taiwan*

TP 223 **Recent Trends in PDE-5 Inhibitors in Consumer Products**; Flavia Morales-garcia[1]; Sara E. Kern[1]; Valerie M. Toomey[1]; Melanie N. Parsons[1]; *[1]US FDA Forensic Chemistry Center, Cincinnati, OH*

TP 224 **Development of a PRM Assay for Detection of Walnut and Hazelnut in Foods**; Justin Marsh[1]; Charles Yang[2]; Melanie Downs[1]; Philip Johnson[1]; *[1]University of Nebraska Lincoln, Lincoln, NE; [2]Thermo Fisher Scientific, San Jose, CA*

TP 225 **Determination of Total Avilamycin Residues in Beef by LC-MS/MS**; Lusha Xu[1]; haijuan an[1]; *[1]Shimadzu (Shanghai) Global Laboratory Consumables Co., Ltd. Beijing Branch, Beijing, China*

TP 226 **The Evaluation of Malachite Green and its Metabolites in Sediments of Aquaculture Environmentin Taiwan**; Lai-Chuan Chang[1]; Tzong-Shean Chin[2]; *[1]Biotech Total Solutions Co., Ltd., New Taipei City, Taiwan; [2]National Chia Yi University Taiwan, Chia Yi City, Taiwan*

TP 227 **Simultaneous Determination of 130 Veterinary Drug in Pork Using Ultra Performance Liquid Chromatograph-Tandem Mass Spectrometry**; Zhao Liu; *Shimadzu (China) Co.,Ltd., Shanghai, China*

TP 228 **Determination of 113 Pesticide Residues in Tea by LC-MS/MS**; Chenyuan Zhang[1]; Haijuan An[2]; Jian Kang[3]; *[1]Shimadzu (Shanghai) Global Laboratory Consumables Co., Ltd., Shanghai, China; [2]Shimadzu (Shanghai) Global Laboratory Consumables Co., Ltd. Beijing Branch, Beijing, China; [3]Shimadzu (Shanghai) Global Laboratory Consumables Co., Ltd., Shanghai, China*

TP 229 **Separation and Quantification of N-Acetyl-Cysteine and Glutathione by Isotopic Iodoacetamide Modification and HILIC Coupled with Tandem Mass Spectrometry**; Shih-shin Liang; *Kaohsiung Medical University, Kaohsiung, Taiwan*

TP 230 **Rapid Screening and Quantitative Analysis of Pesticides in Vegetables by Liquid Chromatography Tandem Quadrupole Time of Flight Mass Spectrometry**; Biao Ren; *Shimadzu(China)Co.,LTD.Beijing Branch, Beijing, China*

TP 231 **Simultaneous Determination of Tebufenozide and Indoxacarb in Animal Products Using Liquid-Liquid Extraction Method Coupled with Liquid Chromatography-Tandem Mass Spectrometry**; Kyung-Hee Yoo[1]; Da-Hee Park[1]; Seong-Kwan Kim[1]; Ho-Chul Shin[1]; *[1]Konkuk university, Seoul, South Korea*

TP 232 **Simultaneous Detection of Eight Prohibited Flavor Compounds in Foodstuffs Using Gas Chromatography–Tandem Mass Spectrometry**; Feng Zhang[1]; Feng Feng[1]; *[1]Institute of Food Safety, Chinese Academy of Inspection and Quarantine, Beijing, China*

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TP 234 **Extractables and Leachables Analysis of Common Household Food Storage Products Using a Quadrupole Time-of-Flight (Q-TOF) Mass Spectrometer**; Evelyn H. Wang[1]; Helen Hao[1]; Gerard Byrne[1]; Jennifer Davis[1]; Katie Pryor[1]; Christopher Gilles[1]; *[1]Shimadzu Scientific Instruments, Inc., Columbia, MD*

TP 235 **Pesticide Residue Analyses of QuEChERS Extracts of Different Food Matrices Using an Online Robotic SPE Clean-up Procedure Coupled to LC-MS/MS**; Michael Hudson; *Thermo Fisher Scientific, San Jose, CA*

TP 236 **Simultaneous Analysis of Multiple Food Allergen and its Detection from Processed Food**; Tairo Ogura[1]; Yuka Fujito[2]; Toshiya Matsubara[1]; Ichiro Hirano[1]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Shimadzu Scientific Instruments, Inc., Columbia, MD*

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TP 238 **A Multiresidue Method for Pesticide Analysis Using an Orbitrap Tribrid Mass Spectrometer and Automatic Background Exclusion**; Anastasia Kalli[1]; Dipankar Ghosh[1]; Seema Sharma[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

TP 239 **Targeted Screening and Quantitation of Pesticide Residues in Green Tea Using a Quadrupole Time-of-Flight Mass Spectrometer**; Toshiya Matsubara[1]; Huan Lin[1]; Natsuyo Asano[1]; Mikie Shima[2]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]AiSTI Science Co., Ltd., Wakayama, Japan*

TP 240 **Simultaneous Determination of Pesticide Residues in Vegetable Extract by Liquid Chromatograph Tandem Mass Spectrometry for High Recovery Rate**; Nozomi Maeshima[1]; Manami Kobayashi[1]; Masuda Junichi[1]; *[1]Shimadzu Corporation, Hadano, Japan*

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TP 242 **Development and Validation of LC-MS/MS Method for Determination of Lipophilic and Hydrophilic Marine Toxins**; Renat Selimov[1]; Ayshat Botasheva[1]; Elizaveta Goncharova[1,2]; Denis Nekrasov[1]; Pavel Metalnikov[1]; Alexandre Komarov[1]; *[1]VGNKI, Moscow, Russian Federation; [2]Moscow State University, Moscow, Russian Federation*

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TP 244 **Determination of Bloodstain Deposition Time Using Metabolomic Analysis**; Hyebin Choi[1]; Ae Eun Seok[2]; Jiyeoug Lee[2]; You-rim Lee[1]; Arum Park[2]; Sora Mun[1]; Yoo-jin Lee[1]; Hyo-jin Kim[1]; Hee-gyoo Kang[1,2]; *[1]Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Daejeon, South Korea; [2]Department of Biomedical Laboratory Science, College of Health Sciences, Eulji University, Seongnam-si, South Korea*

TP 245 **BAC Analysis Utilizing GCMS and FID Combined with Fully Automated Sample Prep Perfomed but Robotic Sampler**; Alan Owens[1]; Rachel Lieberman[2]; Francis Welch[2]; Andy Sandy[2]; *[1]Shimadzu Scientific Instruments, Columbia, MD; [2]Shimadzu Scientific Instruments, Inc., Columbia, MD*

TP 246 **Time of Flight Secondary Ion Mass Spectrometry (TOF-SIMS) Imaging of Illicit Narcotics**; Greg Gillen[1]; Shin Muramoto[2]; Jennifer R. Verkouteren[2]; Edward Sisco[2]; *[1]National Institute of Standards and Technolgoy, Gaithersburg, MD; [2]NIST, Gaithersburg, MD*

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TP 248 **Implementation of an Online µSPE - The Final Step Towards Fully Automated LC-MS Urine Screening in Forensic Toxicology**; Michaela Schmidt[1,2]; Marina Schumacher[3]; Birgit Schneider[3]; Laura M. Huppertz[2]; Jürgen Kempf[2]; *[1]Faculty Medical and Life Sciences, Furtwangen University,, Schwenningen, Germany; [2]Institute of Forensic Medicine, Medical Center – University of Freiburg, Freiburg, Germany; [3]Bruker Daltonik GmbH, Bremen, Germany*

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TP 250 **High-Spatial Resolution Matrix Assisted Laser Desorption/Ionization Mass Spectrometry Imaging of Human Hair Cross-Sections**; Emily C King[1]; Young-Jin Lee[1]; *[1]Iowa State University, Ames, IA*

TP 251 **Method Validation of Drugs of Abuse Using Microchip Capillary Electrophoresis/Mass Spectrometry**; Christopher Nicholson[1]; Sabra Botch-Jones[2]; Scott Miller[1]; Adi Kulkarni[1]; *[1]908 Devices, Boston, MA; [2]Boston University School of Medicine, Boston, MA*

TP 252 **Novel Platform for Online Sample Preparation and LC-MS/MS Analysis of Drugs in Biological Matrices**; Sarah Olive[1]; Joshua Emory[1]; Aria McCall[2]; Ruth Gordillo[3]; Robert English[1]; Rachel Lieberman[1]; Brian Feild[1]; Benjamin Figard[1]; *[1]Shimadzu Scientific Instruments, Inc., Columbia, Maryland; [2]Tarrant County Medical Examiner's Office, Fort Worth, Texas; [3]University of Texas Southwestern Medical School, Dallas, Texas*

TP 253 **A New Method for Species Identification Using Mass Spectrometry and Machine Learning**; Heyi Yang[1]; Erin Butler[1]; Jennifer Teubl[2]; Samantha Monier[1]; David Fenyo[2]; Donald Siegel[1]; *[1]Office of Chief Med Exam, New York, NY; [2]NYU Medical Center, New York, NY*

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TP 255 **Analysis of Drugs and their Metabolites in Human Hair by Online SFE-SFC-MS/MS**; Takahiro Goda[1]; Junichi Masuda[1]; Manami Kobayashi[1]; Maiko Kawamura[2]; Ruri Kikura-Hanajiri[2]; *[1]Shimadzu Corporation, Hadano, Japan; [2]National Institute of Health Sciences, Kawasaki, Japan*

TP 256 **Development of a Screening Method for Illicit Drugs in Hair Using LDTD-MS/MS at 8 Seconds Per Sample**; Sandra Imrazene[1]; Serge Auger[1]; Pier-Luc Plante[2]; Jean Lacoursière[1]; Pierre Picard[1]; *[1]Phytronix Technologies, Quebec, QC; [2]Université Laval, Quebec, Quebec*

TP 257 **Analysis of Synthetic Fentanyl Opioids in Serum Using Captiva EMR-Lipid Sample Preparation by LC-QTOF**; Julie Cichelli; *Agilent Technologies, West Chester, PA*

TP 258 **Methamphetamine Impurity Profiling with GC×GC-TOFMS in Korea**; Beom Jun Ko[1]; Jin Young Kim[1]; Dong Won Shin[1]; *[1]Supreme Prosecutors' Office, Seoul, South Korea*

TP 259 **Screening, Quantification and Confirmation of Fentanyl Metabolite, N-[1-(2-phenethyl-4-piperidinyl)maloanilinic Acid, in Equine Urine for Doping Control Analysis by LC-MS/MS**; Youwen You[1]; Rachel M Proctor[1]; Fuyu Guan[1]; Jaclyn R Missanelli1[1]; Xiaoqing Li[1]; Mary A Robinson[1]; *[1]University of Pennsylvania, Philadephia, PA*

TP 260 **Mass Spectrometry-Based Detection of Genetically Variable Peptides: An Alternative to DNA Typing**; Andrew J Reed[1]; Maryam Baniasad[2]; Stella M Lai[3]; Liwen Zhang[3]; Florian Busch[3]; Vicki H. Wysocki[3]; Myles W Gardner[4]; F. Curtis Hewitt[4]; Michael A. Freitas[3]; *[1]Campus Chemical Instrument Center, Ohio State University, Columbus, OH; [2]The Ohio State University, Columbus; [3]The Ohio State University, Columbus, OH; [4]Signature Science, LLC, Austin, TX*

TP 261 **Sub-minute Analysis for Samples of Forensic Applications**; Luis Cuadra-Rodriquez[1]; Melissa Churley[1]; Lakshmi Krishnan[1]; Courtney Milner[1]; *[1]Agilent Technologies, Inc., Santa Clara, CA*

TP 262 **Identification of Genetically Variable Peptides from Human Skin Samples for Human Forensic Investigation**; Myles W. Gardner[1]; F. Curtis Hewitt[1]; Michael A. Freitas[2]; August E. Woerner[3]; Liwen Zhang[2]; Maryam Baniasad[2]; Kathleen Q. Schulte[1]; Alan R. Smith[1]; Danielle S. LeSassier[1]; Clifton J. Krueger[1]; Nicolette C. Albright[1]; Katharina L. Weber[1]; Tara E. Manley[1]; Leah W. Allen[1]; Megan E. Powals[1]; Benjamin C. Ludolph[1]; *[1]Signature Science, LLC, Austin, TX; [2]The Ohio State University, Columbus, OH; [3]Center for Human Identification, University of North Texas Health Science Center, Fort Worth, TX*

TP 263 **Development of Fiber Spray Ionization Mass Spectrometry (FSI-MS) for Direct Analysis of Drugs in Forensic Samples: A Comparison with PSI-MS**; João Francisco Allochio Filho[1,2]; Nayara Araujo dos Santos[2]; Hanna Leijoto de Oliveira[3]; Keyller Bastos Borges[3]; Valdemar Lacerda Júnior[2]; Wanderson Romão[2,4]; *[1]Federal Institute of Espirito Santo, São Mateus, Brazil; [2]Petroleomic and Forensic Chemistry Laboratory, Department of Chemistry, Federal University of Espirito Santo, Vitória, Brazil; [3]Federal University of São João del-Rei, Department of Natural Sciences, São João del-Rei, Brazil; [4]Federal Institute of Espírito Santo, Vila Velha, Brazil*

TP 264 **Proteomics Can Infer DNA Genotype from a Single Human Hair in Forensic Science**; Glendon Parker[1]; Zachary Goecker[2]; Jennifer Milan[2]; Christina De Leon[2]; Rachel Franklin[2]; Michelle Salemi[2]; Bailey Wills[3]; Brett Phinney[2]; Susan Walsh[3]; Robert Rice[2]; *[1]University of California Davis, Davis, CA; [2]University of California, Davis, Davis, CA; [3]Indiana University-Purdue University Indianapolis, Indianapolis, Indiana*

TP 265 **Determination of Health Status by MALDI-MSI of Latent Fingerprints**; Kelly O'neill[1]; Paige Hinners[1]; Young-Jin Lee[1]; *[1]Iowa State University, Ames, IA*

TP 266 **Forensic Sampling Using Nanoparticle Extraction and Capture**; Jamira A Stephenson[1]; Fabrizio Donnaruma[1]; Kermit K Murray[1]; *[1]Louisiana State University, Baton Rouge, LA*

TP 267 **Rapid In-Situ Analysis of Volatile Organic Compounds from Biological Samples of Forensic Interest**; Stephanie Rankin-Turner; *Loughborough University, Loughborough, United Kingdom*



TP 268 **Modelling Retention Behavior on Analysis of Psychoactive Compounds in Hallucinogenic Mushrooms by HILIC-MS**; Wen Jiang[1]; Norbert Rácz[2]; Júlia Nagy[3]; Tibor Veress[3]; *[1]HILICON AB, Umea, Sweden; [2]Department of Inorganic and Analytical Chemistry, Budapest University of Technology and Economics, Budapest, Hungary; [3]Department of Drug and Arson Investigation, Hungarian Institute for Forensic Sciences, Budapest, Hungary*

TP 269 **Utility of High Resolution Mass Spectrometry (HRMS) for the Discovery of Emerging Synthetic Cannabinoids and their Metabolites in Forensic Casework**; Alex Krotulski[1]; Amanda LA Mohr[1]; Barry K Logan[1,2]; *[1]Center for Forensic Science Research and Education, Willow Grove, PA; [2]NMS Labs, Willow Grove, PA*

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TP 271 **"Understanding" Adduct Ion Molecular Structures and Stability in the Gas-Phase, Improving the Separation Power in Ion Mobility Spectrometry; A View**; Maarten Honing[1]; Darya Hadavi[2]; Jonah Norbury[1]; Marina Borzova[1]; Erik Lange van[1]; *[1]Maastricht Multimodal Molecular Imaging (M4I) Institute, Division of Imaging Mass Spectrometry, Maastricht, Netherlands; [2]Maastricht Multimodal Molecular Imaging (M4I) Institute, Division of Imaging Mass Spectrometry, Maastricht, Netherlands*

TP 272 **Systematic Alteration of Gas-Phase Acidities and Conformations with Insertion of a D-Amino Acid in Oligopeptides**; Yuntao Zhang[1]; Joshua S. Ho[1]; Jianhua Ren[1]; *[1]University of the Pacific, Stockton, CA*

TP 273 **Conformations and Energetics of B- and Y-Ions in Peptoid Fragmentation**; Joshua S. Ho[1]; Yuntao Zhang[1]; Jianhua Ren[1]; *[1]University of the Pacific, Stockton, CA*

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TP 275 **Solely Concentrating on the Negative Aspects of Life**; Jordan Rabus[1]; Philippe Maître[2]; Benjamin J Bythell[3]; *[1]University of Missouri, Saint Louis, MO; [2]Laboratoire de Chimie Physique (UMR8000), CNRS, Univ. Paris-Sud, Université Paris-Saclay, Orsay, France; [3]University of Missouri, St. Louis, MO*

TP 276 **Characterization of Precursor and Product Ions from Copper (II) Cationized, N-terminally Modified Glycine-Glycine Using Infrared Multiple-Photon Photodissociation Spectroscopy**; Susan Kline[1]; Amanda Bubas[1]; Luke J. Metzler[1]; Connor Graca[1]; Theodore Corcovilos[2]; Jonathan Martens[3]; Giel Berden[3]; Jos Oomens[3]; Michael J. Van Stipdonk[1]; *[1]Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA; [2]Department of Physics, Duquesne University, Pittsburgh, PA; [3]Radboud University Nijmegen, Institute for Molecules and Materials, FELIX Facility, Nijmegen, Netherlands*

TP 277 **Spectral Derivatives. Exploring and Exploiting the Collision Energy Dependence of Tandem Mass Spectra**; Yamil Simon; *NIST, Gaithersburg, MD*

TP 278 **Computational Analysis of Tandem-Trapped Ion Mobility / Mass Spectrometry Measurements Relates Identity of Proteoforms to their Tertiary and Quaternary Structures**; Christian Bleiholder[1]; Fanny C Liu[1]; Tyler C Cropley[1]; Mengqi Chai[1]; *[1]Florida State University, Tallahassee, FL*

TP 279 **Dissociation Chemistry In Model Crude Oil Components**; Maha Abutokaikah[1]; Giri R Gnawali[1]; Joseph W Frye[1]; Curtis M Stump[1]; John Tschampel[1]; Christopher D Spilling[1]; Benjamin J Bythell[1]; *[1]University of Missouri, St. Louis, MO*

TP 280 **Structure and Reactivity of Anionic Uranyl Complexes with Acetate and Halide Ligands**; Anna Iacovino[1]; Irena Tatosian[1]; Luke Metzler[1]; Theodore Corcovilos[1]; Giel Berden[2]; Jonathan Martens[2]; Jos Oomens[2]; Michael Van Stipdonk[1]; *[1]Duquesne University, Pittsburgh, PA; [2]Radboud University Nijmegen, Institute for Molecules and Materials, FELIX Facility, Nijmegen, Netherlands*

TP 281 **Experimental and Computational Investigation of the Hydrolysis of Gas-phase [UVIO2(R)]+, R=CH3, CH2CH3, CH=CH2 and C6H5**; Michael J. Van Stipdonk[1]; Irena Tatosian[1]; Amanda Bubas[1]; Anna Iacovino[1]; Susan Kline[1]; Luke Metzler[1]; *[1]Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA*

TP 282 **Probing the Intrinsic Conformation of Anionic Uranyl Complexes Using IRMPD Spectroscopy and Quantum Chemical Calculations**; Scott D. Rissler[1]; Michael J. Van Stipdonk[1]; Luke Metzler[1]; Connor J Graca[1]; Irena Tatosian[1]; Amanda Bubas[2]; *[1]Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA; [2]University of Utah, Salt Lake City, UT*

TP 283 **MultiCRAFTI: Relative Collision Cross Sections Through FTICR Methods without Need for Accurate Pressure Measurements or Single-Collision Dephasing Conditions**; Brigham Pope[1]; Daniel Joaquin[1]; Jacob Hickey[1]; David Dearden[1]; *[1]Brigham Young University, Provo, UT*

TP 284 **Dependence of CRAFTI cross-sections on ion-neutral center-of-mass kinetic energy and ion dissociation energy**; Andrew J. Arslanian[1]; Noah Mismash[1]; Jacob Shaner[1]; Tina H. M. Farzan[1]; Jamir Shrestha[1]; David V. Dearden[1]; *[1]Brigham Young University, Provo, UT*

TP 285 **Determining Topologies of Alkylammonium Complexes of Cucurbit[6]uril Using multiCRAFTI Techniques in an FTICR Mass Spectrometer**; Jamir Shrestha[1]; Zixuan Feng[1,2]; Mariah Pay[1]; Andrew J. Arslanian[1]; Tina H. M. Farzan[1]; Brigham Pope[1]; Jiewen Shen[1]; David V. Dearden[1]; *[1]Brigham Young University, Provo, UT; [2]Colorado State University, Fort Collins, CO*

TP 286 **Structures and Characteristics of Cucurbit[5]uril-Halide Inclusion Complexes Capped by Alkali Metal Cations *via* CRAFTI Collision Cross Sections**; Jiewen Shen[1]; Tina H. M. Farzan[1]; David V. Dearden[1]; *[1]Brigham Young University, Provo, UT*

TP 287 **The Effects of Neutral Guest in Cucurbit[5]uril Complexes Containing Various Metals on its CRAFTI Collision Cross Sections**; Tina H. M. Farzan[1]; Joseph W. Wilson[1]; Sam Hickenlooper[1,2]; Andrew J. Arslanian[1]; David V. Dearden[1]; *[1]Brigham Young University, Provo, UT; [2]University of Utah, Salt Lake City, UT*

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TP 289 **Elucidating H/D-Exchange Mechanism of Active Hydrogen in PAH Compounds**; Arif Ahmed[1]; Syful Islam[1]; Sunghwan Kim[1]; *[1]Kyungpook National University, Daegu, South Korea*

TP 290 **Simulation of Charged Nanodroplets in MS-Transfer-Stage Ion-Guides**; Clara Markert[1]; Walter Wissdorf[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]Bergische Universität Wuppertal, Wuppertal, Germany*

TP 291 **Investigating the Mechanism of Multivalent Cation-Induced Protein Supercharging through MD Simulations and Native MS Experiments**; Leanne Martin[1]; Haidy Metwally[1]; Lars Konermann[1]; *[1]University of Western Ontario, London , ON*

TP 292 **Insights into Ion Release from VSSI Droplets Obtained with Molecular Dynamics Simulations**; Kinkini Udara Jayasundara[1]; Nandhini Ranganathan[1]; Chong Li[1]; Ahmad Kiani Karanji[1]; Peng Li[1]; Stephen Valentine[1]; *[1]West Virginia University.C. Eugene Bennett Department of Chemistry, Morgantown, WV*

TP 293 **The Role of Trace Constituents for the Sustained Operation of Corona Discharges in APCI**; Florian Stappert[1]; Steffen Braekling[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

TP 294 **Systematic Investigations of Electron Ionization Fragmentation Patterns of Selected MOCVD Precursors: Source Temperature and Electron Energy Dependence**; Yessica Brachthäuser[1]; Joshua Rieger[2]; Markus Langner[2]; Alexander Laue[1]; Hin Yiu Chung[1]; Thorsten Benter[2]; *[1]Zeiss SMT GmbH, Oberkochen, Germany; [2]University of Wuppertal, Wuppertal, Germany*

TP 295 **The Mechanism of Carbohydrate Ionization to Form Metal-Ion Adducts from Nanosized Droplets during Electrospray**; Emvia I Calixte[1]; Tara Liyanage[1]; H. Jamie Kim[1]; Emily D. Ziperman[1]; Amanda J Pearson[1]; Elyssia S. Gallagher[1]; *[1]Baylor University, Waco, TX*

TP 296 **Characterization of Ion-Molecule Reactions within Quadrupole Ion Trap Mass Analyzers by Chemical Modification of the Collision Gas**; Christine Polaczek[1]; Marco Thinius[2]; Hendrik Kersten[2]; Thorsten Benter[2]; *[1]University of Wuppertal, Wuppertal, Germany; [2]University of Wuppertal, Wuppertal, Germany*

TP 297 **Numerical Study of Fluid Atomization in a High-Velocity Spray**; Wei Wang[1,2]; Steve Bajic[1]; Benzi John[2]; David R. Emerson[2]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Daresbury Laboratory, Science and Technology Facilities Council, Warrington, United Kingdom*

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TP 299 **A Simple VOC Capturing Method Coupled with GC-MS**; Takeshi Furuhashi[1]; Shigenori Ota[2]; *[1]Anicom Specialty Medicinal Institute Inc, Tokyo, Japan; [2]GL science Inc, Iruma city, Saitama prefecture, Japan*

TP 300 **Tuning the Molecular Ion Abundance in Electron Ionization Mass Spectra and its Effects on Sample Identification**; Ksenia Kladchenko[1]; Alexander B. Fialkov[1]; Tal Alon[1]; Aviv Amirav[1]; *[1]Tel-Aviv University, Tel-Aviv, Israel*

TP 301 **Complementary Techniques in the Environmental GC-MS Analysis**; Albert T Lebedev[1]; Viatcheslav Artaev[2]; Dmitrii Mazur[1]; Georgii Tikhonov[2]; *[1]Moscow State University, Moscow, Russian Federation; [2]LECO Corporation, St Joseph, MI*

TP 302 **Rapid Quantitative Analysis of Melamine in Semi-Solid Food**; Michael D Browne[1]; Tommy Nguyen[1]; Krege Christison[1]; Itsuko Iwai[2]; O. David Sparkman[1]; *[1]University of the Pacific, Stockton, CA; [2]Diablo Analytical, Antioch, CA*

TP 303 **Comprehensive Determination of 209 Polychlorinated Biphenyls Using Two-Dimesional Gas Chromatrgraphy Triple Quadrupole Mass Spectrometry**; Yun Zou[1]; Shizhen Zhao[2]; Gan Zhang[2]; Satoshi Yamaki[1]; Yuki Hashi[3]; Naoki Hamada[1]; *[1]Shimadzu(China)Co.,LTD.Beijing Branch, Beijing, China; [2]Guangzhou Institute of Geochemistry, Chinese Academy of Sciences, Guangzhou, China; [3]Shimadzu (China) Co., LTD., SHANGHAI, China*

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TP 305 **An Optimization Tool for MS Signal Acquisition in GC Triple Quadrupole Mass Spectrometry**; Anastasia Andrianova[1]; Melissa Churley[2]; *[1]Agilent Technologies, Wilmington, DE; [2]Agilent Technologies, Santa Clara, CA*

TP 306 **Volatile Profile Comparison of Flavored and Non-Flavored Vodkas by Purge & Trap Thermal Desorption GC/MS**; Ron Shomo; *Adaptas Solutions, ringoes, NJ*

TP 307 **Open Characterization of Vaping Liquids (e-liquids)**; Ivana Kosarac[1]; Xinghua Fan[1]; Cariton Kubwabo[1]; Wei He[1]; Jun Man[1]; Trevor K. Mischki[1]; *[1]Health Canada, Ottawa, ON*

TP 308 **Flow modulated GCxGC coupled to TOFMS for Non-Target Profiling of Food, Flavor, and Fragrance Samples**; Elizabeth Humston-Fulmer[1]; Lome Fell[1]; Joesph E Binkley[1]; *[1]LECO Corporation, St Joseph, MI*

TP 309 **Tandem Ionisation for Improved Characterisation of Fragranced Products**; Pete Grosshans[1]; Laura McGregor[1]; Nick Bukowski[1]; Gerhard Horner[2]; *[1]SepSolve Analytical, Peterborough, United Kingdom; [2]Five Technologies, Munich, Germany*

TP 310 **Coupling Comprehensive Two-Dimensional Gas Chromatography with an Orbitrap MS for Enhanced Separation and Identification**; Xin Zheng[1]; Jason Cole[2]; *[1]Thermo Fisher Scientific, Austin, TX; [2]Thermo Fisher Scientific, Ausitn, TX*

TP 311 **Qualitative and Quantitative Analysis of Electronic Cigarette Liquids Using Gas Chromatography – Orbitrap Mass Spectrometry**; Jane A Cooper[1]; Chris Allen[2]; Cristian I Cojocariu[1]; Brody Guckenberger[3]; *[1]Thermo Fisher Scientific, Runcorn, United Kingdom; [2]Broughton, Skipton, United Kingdom; [3]Thermo Fisher Scientific, Austin, TX*

TP 312 **Non-Targeted Analysis of Natural Waters with GC-QTOFMS – Addressing Critical Methodological and Data-Evaluation Challenges**; Christina Troyer[1]; Sebastian Handl[1]; Zora Jandric[1]; Kaan Kutlucinar[1]; Tuba Recber[1]; Ernest Mayr[1]; Roza Allabashi[1]; Reinhard Perfler[1]; Stephan Hann[1]; *[1]University of Natural Resources and Life Sciences (BOKU), Vienna, Austria*

TP 313 **Novel GC-MS Ionization Technique to Identify Unknown Compounds**; Riki Kitano[1]; Masato Takakura[2]; Akira Aono[2]; Kouki Tanaka[2]; *[1]Shimadzu Scientific Instruments, Inc., Columbia, Maryland; [2]Shimadzu Corporation, Kyoto, Japan*

TP 314 **Humans Smell to their Skin Microbiome and Microbes Smell Like What They Eat**; Mabel Cristina Gonzalez[1]; Chiara Carazzone[1]; Adriana Marcela Celis[1]; Jorge Alberto Molina[1]; *[1]Universidad de los Andes, Bogota, Colombia*

TP 315 **Highly Sensitive TOF Mass Spectrometer coupled with a New User Friendly Flow Modulator for GCxGC-MS Analysis of Complex Mixtures**; David Jesse Borton[1]; Jonelle Shiel[1]; Mark Merrick[1]; Viatcheslav Artaev[1]; John V Seeley[2]; *[1]LECO Corporation, Saint Joseph, MI; [2]Oakland University, Rochester, MI*

TP 316 **Confident Confirmation of Steroids in Urine by Gas Chromatography-Advanced Electron Ionization (AEI)-Triple Quadrupole Mass Spectrometry**; Gustavo de Albuquerque Cavalcanti[1]; Amit C Gujar[2]; Henrique Marcelo Gualberto Pereira[3]; Francisco Radler de Aquino Neto[4];

Monica Costa Padilha[5, 6]; [1]*Federal University of Rio de Janeiro - UFRJ- Brazilian Doping Control Laboratory -LBCD, Rio de Janeiro, Brazil;* [2]*Thermo Fisher Scientific, Austin, TX;* [3]*Federal University of Rio de Janeiro - UFRJ - Brazilian Doping Control Laboratory -LBCD, Rio de Janeiro, Brazil;* [4]*Federal University of Rio de Janeiro - UFRJ- Brazilian Doping Control Laboratory - LBCD, LADETEC, Rio de Janeiro, Brazil;* [5]*Federal University of Rio de Janeiro - UFRJ- Brazilian Doping Control Laboratory -LBCD,, Rio de Janeiro, Brazil;* [6]*Federal University of Rio de Janeiro - UFRJ- Research Laboratory of Anabolic Agents, LAPAA, Rio de Janeiro, Rio de Janeiro, Brazil, Rio de Janeiro, Brazil*

TP 317 **Molecular-Ion Detection and Fragmentation Mechanisms of a Common Extractable 1,4,7-Trioxacyclotridecane-8,13-dione by GC/HRMS in Electron Ionization and Chemical Ionization Modes**; Chongming Liu[1]; Dujuan Lu[1]; Danny Hower[1]; Xiaoteng Gong[1]; [1]*SGS North America Inc., Fairfield, NJ*

TP 318 **Analysis of Polychlorinated Dibenzo-p-dioxins, Furans and Biphenyls in Drinking Water with Semi-Automated Solid Phase Extraction Using EPA Method 1613**; Rudolf Addink[1]; Tom Hall[1]; [1]*Toxic Report, Watertown, MA*

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TP 320 **Hydrogen Deuterium-Exchange Mass Spectrometry to Measure Nucleosome Dynamics**; Abigail A. Lemmon[1]; Geoffrey P. Dann[1]; Kelly R. Karch[1]; Benjamin A. Garcia[1]; [1]*University of Pennsylvania, Philadelphia, PA*

TP 321 **Conformational Changes of BtuF upon Binding to Vitamin B12 Revealed by Hydrogen Deuterium Exchange Nanospray Mass Spectrometry**; Lijun Zhou; *Nanjing University of science and technology, Nanjing, China*

TP 322 **Active Site Single Point Mutations Modulates the Dynamic Properties of Human Monoacylglycerol Lipase: A Hydrogen Deuterium Exchange Mass Spectrometry Study**; Ioannis Karageorgos[1]; Sergiy Tyukhtenko[2]; Kyle Anderson[1]; Girija Rajarshi[2]; Nikolai Znonok[2]; Alexandros Makriyannis[2]; Jeffrey Hudgens[1]; [1]*NIST, Rockville, MD;* [2]*Northeastern University, Boston, MA*

TP 323 **Integrating HDX-MS and Native MS into Structure-Based Drug Discovery**; Liliana Pedro[1]; Dayana Argoti[1]; Weiping Jia[1]; Patrick Rudewicz[1]; [1]*Novartis Institutes for Biomedical Research, Emeryville, CA*

TP 324 **Hydrogen-Deuterium eXchange Coupled to Mass Spectrometry Highlights a Reciprocal Crosstalk between the Inner and Outer Rings of the 20S Proteasome**; Jean Lesne[1]; Julien Parra[1]; Dusan Zivkovic[1]; Thomas Menneteau[1]; Matthieu Chavent[1]; Marie Locard-Paulet[1]; Marie-Pierre Bousquet-Dubouch[1]; Odile Burlet-Schiltz[1]; Julien Marcoux[1]; [1]*Institut de Pharmacologie et de Biologie Structurale, Université de Toulouse, CNRS, UPS, Toulouse, France*

TP 325 **Temperature and Mutation-Dependent Study of a Model TIM Barrel Domain-Containing Enzyme Performed Using Hydrogen/Deuterium Exchange Mass Spectrometry**; Anthony T. Iavarone[1]; Emily J. Thompson[1]; Judith P. Klinman[1]; [1]*UC Berkeley, Berkeley, CA*

TP 326 **Analysis of Oxidatively Damaged Proteins by H/D Exchange Mass Spectrometry**; Vincent A Saullo[1]; Lars Konermann[2]; [1]*University of Western Ontario, London, ON;* [2]*University of Western Ontario, London , ON*

TP 327 **Connecting Ligand-Induced Dynamics to Potency: Analyzing Anti-Cancer Rexinoids by Hydrogen Deuterium Exchange Mass Spectrometry**; Nathalia Melo[1]; Alla Klyuyeva[1]; Olga V Beliaeva[1]; Natalia Kedishvili[1]; Matthew Renfrow[1]; Peter Prevelige[1]; Venkatram Atigadda[1]; Donald Muccio[1]; [1]*University of Alabama at Birmingham, Birmingham, AL*

TP 328 **HDX-MS Unravels Allosteric Mechanisms that Sequentially Unlock the Sec Translocase for Bacterial Protein Secretion**; Srinath Krishnamurthy[1]; Nikolaos Eleftheriadis[1]; Malvina Papanastasiou[2]; Athina Portaliou[1]; Spyridoula Karamanou[1]; Giorgos Gouridis[1]; Anastassios Economou[1]; [1]*Rega Institute, Dept of Microbiology and Immunology, KU Leuven, Leuven, Belgium;* [2]*Broad Institute, Cambridge, MA*

TP 329 **Probing Histone Tail Interactions in Mononucleosomes by HX-ETD-Orbitrap-MS**; Malvina Papanastasiou[1]; Terry Zhang[2]; James Mullahoo[1]; Samuel A. Myers[1]; Steven A. Carr[1]; Jacob D. Jaffe[1]; [1]*Broad Institute, Cambridge, MA;* [2]*Thermo Fisher Scientific, San Jose, CA*

TP 330 **Pulsed Unfolding, HDX, and Digestion of APOE Proteins by Mass Spectrometry Provides Insight into Forcing the Folded Monomeric Species**; Elizabeth T Schaper Bergman[1]; Michael L Gross[1, 2]; [1]*Washington University, St. Louis, MO;* [2]*Washington University School of Medicine, St. Louis, MO*

TP 331 **Covariation Analysis Reveals Functional Regions of RORγ with Concerted Motions**; Tim Strutzenberg; *The Scripps Research Institute, Palm Beach Gardens, FL*

TP 332 **Conformational Preferences for the Tec-Family Tyrosine Kinase BTK in Binding to the HIV-1 Accessory Protein Nef**; Thomas E. Wales[1]; Raji E. Joseph[2]; Shoucheng Du[3]; Thomas E. Smithgall[3]; Amy H. Andreotti[2]; John R. Engen[1]; [1]*Northeastern University, Boston, MA;* [2]*Iowa State University, Ames, IA;* [3]*University of Pittsburgh School of Medicine, Pittsburgh, PA*

TP 333 **Uncovering Differential Effects of IgG Subclasses on Whole DENV Particles with Hydrogen-Deuterium Exchange Mass Spectrometry**; Xin-Xiang Lim[1]; Ganesh S. Anand[1]; [1]*National University of Singapore, Singapore, Singapore*

TP 334 **A Bacterial Flavin-Dependent Oxidoreductase that Undergoes Conformational Changes to Capture Carbon Dioxide**; Jenna Mattice[1]; Bennett Streit[1]; Luke Berry[1]; John Peters[2]; Jennifer DuBois[1]; Brian Bothner[1]; [1]*Montana State University, Bozeman, MT;* [2]*Washington State University, Pullman, WA*

TP 335 **Revealing the Impact of Biological Substrate and Drug Ligands on the Conformational Dynamics of the Human Serotonin Transporter Using HDX-MS**; Ingvar R. Möller[1]; Marika Slivacka[1]; Anne Kathrine Nielsen[2]; Søren G.F. Rasmussen[3]; Ulrik Gether[3]; Claus J. Loland[2]; Kasper D. Rand[1]; [1]*Protein Analysis Group, Department of Pharmacy, University of Copenhagen, Copenhagen, Denmark;* [2]*Laboratory for Membrane Protein Dynamics, Department of Neuroscience, University of Copenhagen, Copenhagen, Denmark;* [3]*Department of Neuroscience, University of Copenhagen, Copenhagen, Denmark*

TP 336 **Probing Protein Ligand Interactions through an Offline MALDI-MS based Hydrogen Deuterium Exchange Study**; Laxmi Sinduri Vuppala[1]; Theresa Evans-Nguyen[1]; Ioannis Gelis[1]; John M. Koomen[1, 2]; [1]*University of South Florida, Tampa, FL;* [2]*Moffitt Cancer Center & Research Institute, Tampa, FL*

TP 337 **HDX-MS Reveals Allosteric Changes in Subtilisin Serine Protease Upon Inhibitor Binding**; Daniel W Pedersen[1, 2]; Jeppe C Mouritsen[1]; Stuart Pengelley[3]; Detlev Suckau[3]; Thomas J D Jørgensen[2]; Christian I Jørgensen[1]; [1]*Novozymes A/S, Bagsværd, Denmark;* [2]*University of*

Southern Denmark, Odense, Denmark; [3]Bruker Daltonik GmbH, Bremen, Germany

TP 338 **Probing Copper Binding in Orange Carotenoid Protein by Using H/DX and Native Mass Spectrometry**; Haijun Liu[1]; Ming Cheng[2]; Jing Yan[1]; Chunyang Guo[1]; Andy Xu[1]; Michael L Gross[1]; Robert E Blankenship[1]; *[1]Washington University, St.louis, MO; [2]Washington University, St Louis, MO*

TP 339 **Thermodynamic Insight for the Formulation Optimization of a Therapeutic Antibody by HDX-MS Analysis and nanoDSF**; Yoshitomo Hamuro[1]; Mehabaw Derebe[1]; Jennifer F. Nemeth-Seay[1]; *[1]Janssen Research and Development, Spring House, PA*

TP 340 **Gas-Phase Hydrogen Deuterium Exchange Coupled with Dissociation of Enkephalin Variants to Investigate Exchange Mechanism**; Cynthia M Suarez[1]; Rebecca A Jockusch[1]; *[1]University of Toronto, Toronto, ON*

TP 341 **Discovery and Characterization of a Synthetic Antigen Binding Fragment (sFab) Inhibiting Marburg Viral RNA Synthesis Incorporating HDX-MS Analyses**; Nicole D. Wagner[1]; Parmeshwar Amatya[2]; Gang Chen[3]; Priya Luthra[4]; Liuqing Shi[1]; Alevtina Pavlenco[3]; Dominika Borek[5]; Henry Rohrs[1]; Christopher F. Basler[4]; Gaya Amarasinghe[2]; Sachdev Sidhu[3]; Michael L Gross[1]; Daisy Leung[2]; *[1]Washington University, St. Louis, MO; [2]Washington University School of Medicine, St. Louis, MO; [3]University of Toronto, Toronto, Ontario; [4]Georgia State University, Atlanta, GA; [5]UT Southwestern Medical Center, Dallas, TX*

TP 342 **Higher-Order Structural Analysis of Pro-Survival BAG-1S through HDX-MS**; Ozge Tatli[1, 2]; Miray Turk[1]; Gizem Dinler Doganay[1]; *[1]Istanbul Technical University, Istanbul, Turkey; [2]Istanbul Medeniyet University, Istanbul, Turkey*

TP 343 **Cyclic AMP-PKA Signalosome Dynamics by HDXMS and Fluorescence Polarization Reveals Regulatory AMP Oscillations**; Nikhil K Tulsian[1, 2]; Abhijeet Ghode[1]; Ganesh S Anand[1]; *[1]Dept. of Biological Sciences, National University of Singapore, Singapore, Singapore; [2]Dept. of Biochemistry, National University of Singapore, Singapore*

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TP 345 **Development and Application of Ambient Mass Spectrometry Images for Dermal Melamine Exposures in Melamine Tableware Manufacturing Workers**; Yu-Ming Hsu[1]; Jentaie Shiea[1, 2]; Ming-Tsang Wu[1, 3, 4]; *[1]Research Center for Environmental Medicine, Kaohsiung Medical University, Kaohsiung, Taiwan; [2]Department of Chemistry, National Sun Yat-sen University, Kaohsiung, Taiwan; [3]Department of Public Health, College of Health Sciences, Kaohsiung Medical University, Kaohsiung, Taiwan; [4]Department of Family Medicine, Kaohsiung Medical University Hospital, Kaohsiung Medical University, Kaohsiung, Taiwan*

TP 346 **Investigation of Chemical Complexity and Cellular Heterogeneity of Human Pancreatic Islets Using Cross-Platform Mass Spectrometric Approach**; Stanislav Rubakhin[1]; Elena V. Romanova[2]; Jonathan V. Sweedler[2]; *[1]Beckman Institute, UIUC, Urbana, IL; [2]University of Illinois at Urbana-Champaign, Urbana, IL*

TP 347 **Developing a Drug Screening Platform: MALDI-Mass Spectrometry Imaging of Paper-Based Cultures**; Fernando Tobias[1]; Gabriel J. LaBonia[2]; Julie McIntosh[3]; Matthew R. Lockett[3]; Amanda B. Hummon[1]; *[1]Department of Chemistry and Biochemistry, Comprehensive Cancer Center, The Ohio State University, Columbus, Ohio; [2]Department of Chemistry and Biochemistry, University of Notre Dame, Notre Dame, Indiana; [3]Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC*

TP 348 **Optimisation of a Bottom-Up Strategy to Detect Biopharmaceuticals in 3D Tumour Models Using MALDI-MSI**; Lucy E Flint[1]; Neil A Cross[1]; Laura M Cole[1]; David P Smith[1]; Malcolm R Clench[1]; *[1]Sheffield Hallam University, Sheffield, United Kingdom*

TP 349 **Utilizing Formalin Fixation for Enhancing Detection of Neuropeptides from the Crustacean Brain by MALDI-MS Imaging**; Nhu Q. Vu[1]; Amanda R. Buchberger[1]; Jillian Johnson[1]; Lingjun Li[1]; *[1]University of Wisconsin - Madison, Madison, WI*

TP 350 **Identifying Biomarkers by High Throughput Screening on FFPE Breast Cancer TMAs Using DESI-MSI**; Ólöf Gerdur Ísberg[1]; Dipa Gurung[1]; James McKenzie[1]; Hiromi Kudo[1]; Jon G Jonasson[2]; Sigridur Klara Bodvarsdottir[3]; Margret Thorsteinsdottir[3]; Zoltan Takats[1]; *[1]Imperial College, London, United Kingdom; [2]Landspitali, University Hospital, Reykjavik, Iceland; [3]University of Iceland, Reykjavik, Iceland*

TP 351 **Click Chemistry Driven Fluorophore Addition Allows for Spatial Identification of Liposomal Drug Delivery System Components by MALDI-MSI and Fluorescence Microscopy**; William Andrews; *University of Notre Dame, Notre Dame; The Ohio State University, Columbus, OH*

TP 352 **Mass Spectrometry Imaging of the *in situ* Drug Release from Nanocarriers**; Jinjuan Xue[1]; Huihui Liu[1]; Suming Chen[2]; Caiqiao Xiong[1]; Lingpeng Zhan[1]; Jie Sun[1]; Zongxiu Nie[1]; *[1]Institute of Chemistry, Chinese Academy of Sciences, Beijing, China; [2]Wuhan University, Wuhan, China*

TP 353 **A Tool to Visualize Soil Microbial Community Dynamics Using Mass Spectrometry Imaging and Confocal Microscopy**; Arunima Bhattacharjee[1]; Thomas W Wietsma[1]; Dusan Velickovic[1]; Sheryl L Bell[1]; Janet K Jansson[1]; Kirsten S Hofmockel[1]; Christopher R Anderton[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

TP 354 **An Elegant Approach for Broad Molecular Imaging of the Root-Soil Interface *via* Indirect MALDI-FTICR-MSI**; Dusan Velickovic[1]; Vivian Lin[1]; Albert Rivas[1]; Christopher Anderton[1]; James Moran[1]; *[1]Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA*

TP 355 **The Combination of DIUTHAME-IMS/FT-ICR Conserves High Mass Accuracy and Resolution over the DIUTHAME-IMS/TOFMS in the Laser Desorption/ Ionization Imaging Mass Spectrometry**; Hasan Md. Mahmudul[1]; Yasuhide Naito[2]; Masahiro Kotani[3]; Takayuki Ohmura[3]; Mamun Md. Al[1]; Shumpei Sato[1]; Ariful Islam[1]; A s m Waliullah[1]; Takashi K Ito[1]; Mitsutoshi Setou[1, 4, 5]; *[1]International Mass Imaging Center and Department of Cellular and Molecular Anatomy, Hamamatsu University School of Medicine, Hamamatsu, Japan; [2]The Graduate School for the Creation of New Photonics Industries, Hamamatsu, Japan; [3]Hamamatsu Photonics K.K., Iwata, Japan; [4]Preeminent Medical Photonics Education & Research Center, Hamamatsu, Japan; [5]Department of Anatomy, The University of Hong Kong, Pokfulam, China*

TP 356 **Combination of the Low Vacuum MALDI-Orbitrap Imaging with the Hydrogen/Deuterium Exchange Approach**; Gleb Vladimirov[1]; Yury kostyukevich[1]; Eugene (evgeny) Nikolaev[2]; *[1]Skolkovo Institute of Science and Technology, Skolkovo, Russian Federation; [2]Skolkovo institute of science and technology, Moscow Region, Russian Federation*

TP 357 **Direct Atmospheric Pressure Laser Desorption Ionization for Mass Spectrometry Imaging**; Jing Yang[1]; Wenpeng Zhang[1, 2]; Wenbo Cao[1]; Xiaoxiao Ma[1]; Zheng Ouyang[1]; *[1]State Key Laboratory of Precision Measurement Technology and Instruments, Department*

of Precision Instruments, Tsinghua University, Beijing, China; [2]Department of Chemistry, Purdue University, West Lafayette, IN

TP 358 **Unsaturated Lipid Isomer Distribution Analysis by MALDI MS Imaging with m-CPBA Epoxidation and CID-MS/MS**; Meng Xu[1]; Yu Feng[2]; Lingjun Li[1,2]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI*

TP 359 **Development of Blotting Method Using DIUTHAME for Imaging MS**; Masahiro Kotani[1]; Takayuki Ohmura[1]; Akira Tashiro[1]; Hirofumi Enomoto[2]; Yasuhide Naito[3]; *[1]Hamamatsu Photonics K.K., Iwata, Japan; [2]Teikyo University, Utsunomiya, Japan; [3]The Graduate School for the Creation of New Photonics Industries, Hamamatsu, Japan*

TP 360 **Brimstone Chemistry under Laser Light Assists Mass Spectrometric Detection and Imaging the Distribution of Arsenic in Minerals**; Zhaoyu Zheng[1]; Swapnil Lal[2]; Athula Attygalle[1]; *[1]Stevens Institute of Technology, Weehawken, NJ; [2]Montgomery High School, Skillman, NJ*

TP 361 **Optimizing the Mass Accuracy for Automated Analysis of MALDI Images**; Sophie Rappe[1]; Mathieu Tiquet[1]; Raphaël La Rocca[1]; Johann Far[1]; Loïc Quinton[1]; Gauthier Eppe[1]; Edwin A De Pauw[1]; *[1]Mass Spectrometry Laboratory, MolSys Research Unit, University of Liege, Liege, Belgium*

TP 362 **Optimizing Tissue Ablation for Mass Spectrometry Imaging Using Light Scattering**; Achala P Deenamulla Kankanamalage[1]; Fabrizio Donnaruma[1]; Kermit K Murray[1]; *[1]Louisiana State University, Baton Rouge, LA*

TP 363 **Pulsed Cold Plasma for Post Ionization in MALDI-MS imaging**; Jens Soltwisch[1,2]; Ulrich Röhling[3]; Klaus Dreisewerd[1,2]; *[1]Institute for Hygiene, University of Münster, Münster, Germany; [2]Interdisciplinary Center for Clinical Research (IZKF), University of Münster, Münster, Germany; [3]Institute of Medical Physics and Biophysics, University of Münster, Münster, Germany*

TP 364 **Improving the Mass Range and Field of View in Ion Microscope Imaging Mass Spectrometry**; Natasha M Smith[1]; Fei Gao[1]; Ang Guo[1]; Michael Burt[1]; Robert Burleigh[1]; Mark Brouard[1]; *[1]University of Oxford, Oxford, United Kingdom*

IMAGING MS: PHARMACEUTICAL APPLICATIONS
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TP 365 **Implementing Multi-modal Imaging Platform for Tissue Distribution, Metabolite Profiling and Quantification of Peptide Therapeutics**; Bingming Chen[1]; Marissa Vavrek[1]; Wendy Zhong[2]; Richard Gundersdorf[1]; Bernard Choi[2]; Scott Fauty[1]; Mark Cancilla[1]; *[1]Merck & Co., Inc., West Point, PA; [2]Merck & Co., Inc., Rahway, NJ*

TP 366 **Quantitative Mass Spectrometry Imaging of Diclofenac and its Metabolites in Tissues Using Nanospray Desorption Electrospray Ionization Mass Spectrometry**; Hilary Brown[1]; Bingming Chen[2]; Mark Cancilla[2]; Elizabeth Pierson[3]; Marissa Vavrek[2]; Wendy Zhong[3]; Julia Laskin[1]; *[1]Purdue University, West Lafayette, IN; [2]Merck & Co., Inc., West Point, PA; [3]Merck & Co., Inc., Rahway, NJ*

TP 367 **Investigation of Drug Localization in the Intestinal Tract Using Imaging Mass Spectrometry**; Kerri Grove[1]; Shaila Hoque[1]; Suresh Lakshminarayana[1]; Ying-Bo Chen[1]; Imad Hanna[2]; Joe Young[1]; Ujjini Manjunatha[1]; Patrick Rudewicz[1]; *[1]Novartis Institutes for BioMedical Research, Emeryville, CA; [2]Novartis, Cambridge, MA*

TP 368 **Measurement of Temporal Changes in the Distribution of Imiquimod Administrated Transdermally to Mouse Skin Tissue Using Imaging Mass Spectrometry**; Yuki Fukui[1]; Hisanao Hazama[1]; Taiki Yamasaki[1]; Sayami Ito[1]; Naoki Okada[1]; Kunio Awazu[1]; *[1]Osaka University, Suita, Japan*

TP 369 **The Spheroid Microarray: Pushing *in vitro* Drug Penetration Towards High-Throughput Technologies**; Jillian Johnson[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

TP 370 **Mouse Brain Drug Exposure by Imaging Mass Spectrometry and its Correlation to Whole Brain Pharmacodynamic Parameters**; John Bowling[1]; Alireza Abdolvahabi[1]; Xiang Fu[1]; Lei Yang[1]; Zoran Rankovic[1]; *[1]St. Jude Children's Research Hospital, Memphis, TN*

TP 371 **Metabolomic Studies of Amyloid Plaques in Mouse Brain with Alzheimer Disease Using Mass Spectrometry Imaging Strengthened by Image Fusion**; Xiang Tian[1]; Zhu Zou[1]; Boer Xie[2]; Junmin Peng[2]; Zhibo Yang[1]; *[1]University of Oklahoma, Norman, OK; [2]St.Jude Children's Research Hospital, Memphis, TN*

TP 372 **Development of a Detection Method for Antisense Oligonucleotides in Mouse Livers and Kidneys by MALDI Imaging Mass Spectrometry**; Hiroyuki Yokoi[1,2]; Yuuya Kasahara[3]; Satoshi Obika[2,3]; Takefumi Doi[2]; Haruhiko Kamada[3]; *[1]Otsuka Pharmaceutical Co., Ltd, Tokushima, Afghanistan; [2]Graduate School and School of Pharmaceutical Sciences, Osaka University, Osaka, Japan; [3]National Institute of Biomedical Innovation, Health and Nutrition, Osaka, Japan*

TP 373 **Comparative Study of Pancreatic Insulin and N-Glycans between Lean and Obese Zucker Rats by MALDI Imaging Mass Spectrometry**; Bin Wang[1]; Yatao Shi[1]; Zihui Li[2]; Xudong Shi[3]; Nannan Tao[4]; Lingjun Li[1,2]; *[1]School of Pharmacy, University of Wisconsin-Madison, Madison, WI 53705; [2]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [3]Department of Surgery, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI; [4]Bruker Scientific, LLC, San Jose, CA*

TP 374 **MALDI-Ion Mobility Mass Spectrometry Imaging for Paclitaxel Nanomedcine Distribution in Solid Tumor Tissue**; Bo Wen[1]; Hebao Yuan[1]; Lipeng Dai[1]; Krishani Rajanayake[1]; Miao He[1]; Manjunath Pai[1]; Duxin Sun[1]; *[1]University of Michigan, Ann Arbor, MI*

TP 375 **Different MALDI Mass Spectrometry Imaging Applications on a Prototype MALDI-Q-TOF Instrument**; Janina Oetjen[1]; Alice Ly[1]; Arne Fuetterer[1]; Juergen Suetering[1]; Niels Goedecke[1]; Richard R Drake[2]; Anand Mehta[2]; Michael Becker[3]; Rita Casadonte[4]; Jörg Kriegsmann[4]; Jens Fuchser[1]; Lucy Woods[1]; Oliver Raether[1]; Jens Hoehndorf[1]; Shannon Cornett[5]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Medical University of South Carolina, Charleston, SC; [3]Boehringer Ingelheim Pharma GmbH & Co. KG, Department of Drug Discovery Sciences, Biberach an der Riss, Germany; [4]Proteopath, Trier, Germany; [5]Bruker Daltonics Inc., Billerica, MA*

TP 376 **ToF-SIMS Depth Profiling of Oral Drug Delivery Films for 3D Visualization and Quantification of Active Pharmaceutical Particles**; Shin Muramoto[1]; Greg Gillen[2]; Cayla Collett[2]; *[1], Gaithersburg, MD; [2]National Institute of Standards and Technology, Gaithersburg, MD*

TP 377 ***in-situ* Drug Release Monitoring Using Quantitative 3D Mass Spectrometry Imaging for a Drug Delivery Stent Formulation Optimization**; Lauranne Poncelet[1,2]; Rima Ait-Belkacem[1]; Justine Mougin[2]; Mickael Maton[2]; Dyhia Kersani[2]; Bernard Martel[2]; Stephanie Degoutin[2]; Feng Chai[2]; Nicolas Blanchemain[2]; Jonathan Stauber[3]; *[1]Imabiotech, Loos, France; [2]Université de Lille, Lille, France; [3]ImaBiotech Corp, Boston, MA*

TP 378 **Gadolinium Deposition from MRI Contrast Agents in the Human Body Unraveled by MS Imaging and Speciation Analysis**; Uwe Karst; *University of Münster, Münster, Germany*

TP 379 **MALDI Imaging Studies of Cisplatin Distribution in Mouse Brain Sections**; Hay-Yan J Wang[1,2]; Yi-Feng Dai[2]; Hung-Wei Yang[3]; Chiung-Yin Huang[4]; Kuo-Chen Wei[4]; *[1]Department of Biological Sciences, National Sun Yat-sen University, Kaohsiung, Taiwan; [2]Doctoral Degree Program in Marine Biotechnology, National Sun Yat-sen University and Academia Sinica, Kaohsiung, Taiwan; [3]Institute of Medical Science and Technology, National Sun Yat-sen University, Kaohsiung, Taiwan; [4]Department of Neurosurgery, Linko Chang Gung Memorial Hospital, Taoyuan City, Taiwan*

IMAGING MS: SAMPLE PREPARATION
380-387

TP 380 **Keeping the Shape of Plant Tissue for Visualizing Metabolite Features of Imaging Mass Spectrometry in *Asparagus officinalis***; Ryo Nakabayashi[1]; Kei Hashimoto[1]; Kiminori Toyooka[1]; Tetsuya Mori[1]; Takashi Nirasawa[2]; Kazuki Saito[1,3]; *[1]RIKEN Center for Sustainable Resource Science, Yokohama, Japan; [2]Bruker Japan K. K., Yokohama, Japan; [3]Chiba University, Chuo-ku, Japan*

TP 381 **Creating Normalcy Classifications in Human Kidney Tissue *via* LC-MS/MS Proteomic Analysis for 3-D Molecular Imaging**; Jamie Allen[1,2]; Danielle Gutierrez[1,2]; Maya Brewer[3]; Nathan Heath Patterson[1,2]; Raf Van de Plas[1,2,4]; Mark Decaestecker[3]; Raymond C Harris[3]; Agnes B Fogo[5]; Richard M. Caprioli[1,2,6]; Jeffrey Spraggins[1,2,6]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Vanderbilt University Department of Biochemistry, Nashville, TN; [3]Vanderbilt University Medical Center, Department of Medicine, Nashville, TN; [4]Delft University of Technology, Delft, Netherlands; [5]Vanderbilt University Medical Center Department of Pathology, Microbiology and Immunology, Nashville, TN; [6]Vanderbilt University Department of Chemistry, Nashville, TN*

TP 382 **Understanding and Decreasing Visceral Fat Delocalisation in Imaging Mass Spectrometry**; Frédéric Fournelle[1]; Ethan Yang[1]; Martin Dufresne[2]; Pierre Chaurand[1]; *[1]University of Montreal, Montreal, QC; [2]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN*

TP 383 **Comprehensive Evaluation of Zinc Oxide Nanoparticles as Matrix for MALDI MS Tissue Imaging of Metabolites**; Chaochao Chen[1]; Ken K.-C. Yeung[1]; *[1]University of Western Ontario, London , ON*

TP 384 **Development of Sample Preparation Method to Improve Sensitivity and Reproducibility of Mass Spectrometry Imaging of Endogenous Metabolites**; Tomomi Morikawa-Ichinose[1]; Yoshinori Fujimura[1]; Fusa Murayama[1]; Yuzo Yamazaki[2]; Takushi Yamamoto[2]; Hiroyuki Wariishi[1]; Daisuke Miura[1,3]; *[1]Kyushu University, Fukuoka, Japan; [2]Shimadzu corp., Kyoto, Japan; [3]National Institute of Advanced Industrial Science and Technology, Ibaraki, Japan*

TP 385 **MALDI Imaging of Ocular Lens Cytoskeletal Proteins**; Zhen Wang[1]; Daniel J Ryan[1]; Kevin L Schey[1]; *[1]Vanderbilt University, Nashville, TN*

TP 386 **Combining Mass Spectrometry Imaging and Top-Down Proteomics to Predict Immunotherapy Response in Non-Small-Cell Lung Cancer (NSCLC) Patients**; Eline Berghmans[1,2]; Karin Schildermans[1,2]; Kurt Boonen[1,2]; Patrick Pauwels[3]; Geert Baggerman[1,2]; *[1]Centre for Proteomics (University of Antwerp/VITO (Belgium)), Antwerpen, Belgium; [2]Unit Enviromental Risk & Health, VITO, Mol, Belgium; [3]Department of Pathology, Antwerp University Hospital, Edegem, Belgium*

TP 387 **Biomarker Discovery for Radiation-Induced Lung Injury by Matrix Assisted Laser Desorption/Ionization-Mass Spectrometry Imaging (MALDI-MSI) Using Formalin-Fixed Paraffin-Embedded Tissues**; Ning Pan Bernhardt[1]; Maureen A Kane[1]; *[1]University of Maryland Baltimore School of Pharmacy, Baltimore, MD*

IMAGING MS: SMALL MOLECULES
388-407

TP 388 **Spatial Lipidomics Reveals Altered Lipid Profiles in Glomeruli of Human Diabetic Kidney**; Guanshi Zhang[1,2]; Dušan Veličković[3]; Viktor Drel[1,2]; Sanjay Jain[4]; Shweta Bansal[1,2]; Manjeri A. Venkatachalam[1]; Hongping Ye[1]; Madesh Muniswamy[1]; Xianlin Han[1]; Ljiljana Paša-Tolić[3]; Theodore Alexandrov[5,6]; Christopher Anderton[3]; Kumar Sharma[1,2]; *[1]University of Texas Health-San Antonio, San Antonio, TX; [2]South Texas Veterans Health Care System, San Antonio, TX; [3]Pacific Northwest National Laboratory, Richland, WA; [4]Washington University, St. Louis, MO; [5]European Molecular Biology Laboratory, Heidelberg, Germany; [6]University of California San Diego, La Jolla, CA*

TP 389 **Development of Bimetallic Nanoparticles for Surface-Assisted Laser Desorption/Ionisation Mass Spectrometry Imaging of Small Molecules**; Alexandre Verdin[1]; Cédric Malherbe[1]; Virginie Bertrand[1]; Edwin De Pauw[1]; Gauthier Eppe[1]; *[1]University of Liege, MS Lab - GIGA, MolSys Research Unit, Liege, Belgium*

TP 390 **A Combination of Unroofing and Chemical Fixation Enable TOF-SIMS to Observe the Intracellular Fatty Acid Distribution**; Makoto Horikawa[1,2]; Shiro Takei[3]; Chi Zhang[1]; Setou Mitsutoshi[1,2]; *[1]Department of Cellular & Molecular Anatomy, Hamamatsu University School of Medicine, Hamamatsu, Japan; [2]International Mass Imaging Center, Hamamatsu University School of Medicine, Hamamatsu, Japan; [3]Department of Environmental Biology, College of Bioscience and Biotechnology, Chubu University, Kasugai, Japan*

TP 391 **Subcellular Imaging of Cardiolipin and Phosphatidylethanolamine Using GCIB-ToF-SIMS**; L.J. Sparvero[1,2]; Hua Tian[3]; Andrew Amoscato[1,2]; Simon Watkins[4]; Nicholas Winograd[3]; Valerian Kagan[1,2,5,6]; Hülya Bayır[1,2,7]; *[1]University of Pittsburgh -- EOH Department, Pittsburgh, PA; [2]Center for Free Radical and Antioxidant Health, Pittsburgh, PA; [3]Pennsylvania State University -- Chemistry Department, University Park, PA; [4]University of Pittsburgh -- Departments of Cell Biology and Immunology, Pittsburgh, PA; [5]University of Pittsburgh, Departments of Chemistry, Pharmacology and Chemical Biology, Radiation Oncology, Pittsburgh, PA; [6]Lab of Navigational Redox Lipidomics,IM Sechenov Moscow State Medical University, Moscow, Russia; [7]University of Pittsburgh -- Department of Critical Care Medicine and Safar Center for Resuscitation Research, Pittsburgh, PA*

TP 392 **High Speed, High Lateral Resolution Lipid Imaging in a MALDI-Q-TOF**; Janina Oetjen[1]; Arne Fuetterer[1]; Juergen Suetering[1]; Niels Goedecke[1]; Sören-Oliver Deininger[1]; Lucy Woods[1]; Oliver Raether[1]; Jens Hoehndorf[1]; Shannon Cornett[2]; Jens Fuchser[1]; Nikolas Kessler[1]; Heiko Neuweger[1]; Alice Ly[1]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Bruker Daltonics Inc., Billerica, MA*

TP 393 **Embryo Transfer Change the Spatiotemporal Lipid Signaling during the Early Stage Embryogenesis**; Stefania Gitta[1]; Janos Schmidt[1]; Laszlo Mark[1]; *[1]Institute of Biochemistry and Medical Chemistry, University of Pecs, Pecs, Hungary*

TP 394 **Mapping Lipids in Whole-Body Zebrafish Sections Using IR-MALDESI**; Whitney L Stutts[1]; Megan M Knuth[1]; Mäns Ekelöf[1]; Debabrata Mahapatra[1]; Seth W Kullman[1]; David C Muddiman[1]; *[1]North Carolina State University, Raleigh, NC*

TP 395 **Analysis of Cuttlefish Skin Chromatophores Using a Combination of High Resolution 3D-LDI-MS-Imaging and LC-UV-MS**; Jakob Meier-Credo[1,2]; Jessica S. Eberle[2]; Marcel A. Lauterbach[2]; Sam Reiter[2]; Gilles Laurent[2]; Julian D. Langer[1,2]; *[1]MPI for Biophysics, Frankfurt Am Main, Germany; [2]Max Planck Institute for Brain Research, Frankfurt am Main, Germany*

TP 396 **Spatial Distribution of Endogenous Molecules in Coffee Bean by Atmospheric Pressure Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry Imaging**; Honggang Nie[1]; Chenglong Dong[2]; Yehua Han[2]; Huwei Liu[1]; *[1]Beijing National Laboratory for Molecular Sciences, Peking University, Beijing, China; [2]State Key Laboratory of Heavy Oil Processing, China University of Petroleum, Beijing, China*

TP 397 **Mass Spectrometry Imaging of Dichloroacetate for Evaluating the Effects of Thermoembolization *in-vivo* with CT Correlation**; Dodge Baluya[1]; Chunxiao Guo[1]; Elizabeth Whitley[1]; Erik Cressman[1]; *[1]UT MD Anderson, Houston, TX*

TP 398 **MALDI Imaging of Anti Tuberculosis Drugs with High Mass and Spatial Resolution in Mouse Model Tissue**; Axel Treu[1]; Julia Kokesch-Himmelreich[1]; Kerstin Walter[2]; Christoph Hölscher[2]; Andreas Römpp[1]; *[1]University of Bayreuth, Bayreuth, Germany; [2]Research Center Borstel, Borstel, Germany*

TP 399 **Multimodal Analysis through Mass Spectrometry Imaging and Multi-energy Tomography Using Cesium as an Integrative Marker**; Dodge Baluya[1]; Emily A. Thompson[1]; Megan C. Jacobsen[1]; Rick R. Layman[1]; Elizabeth Whitley[1]; Erik Cressman[1]; *[1]MD Anderson Cancer Center, Houston, TX*

TP 400 **High-Resolution Nano-DESI Mass Spectrometry Imaging for Skeletal Muscle Fiber Analysis**; Daisy M Unsihuay Vila[1]; Feng Yue[2]; Jiamin Qiu[2]; Shihuan Kuang[2]; Ruichuan Yin[1]; Julia Laskin[1]; *[1]Department of Chemistry, Purdue University, West Lafayette, IN 47907; [2]Department of Animal Sciences, Purdue University, 901W State Street, West lafayette, IN*

TP 401 **Quantitative Mass Spectrometry Imaging of Eicosanoids Provides Novel Biological Insights into Premature Birth**; Kyle D. Duncan[1]; Wenbo Deng[2]; Xiaofei Sun[2]; Lisa M. Bramer[4]; Bobbie-jo M. Webb-robertson[3]; Jennifer Kyle[3]; Erin S. Baker[4]; Kristin E. Burnum-Johnson[3]; Sudhansu K. Dey[2]; Ingela Lanekoff[1]; *[1]Uppsala University, Uppsala, Sweden; [2]Division of Reproductive Sciences, Cincinnati Children's Hospital Medical Center, Cincinnati, OH; [3]Biological Sciences Division, Pacific Northwest National Laboratory, Richland, WA; [4]Department of Chemistry, North Carolina State University, Raleigh, NC*

TP 402 **Quantitative Imaging Mass Spectrometry of Endogenous Metabolites Using In-Line Internal Standards and Stable Isotope Labeled Mimetic Model**; Bindesh Shrestha[1]; Khaja Muneeruddin[2]; Scott A Shaffer[2]; *[1]Waters Corp., Beverly, MA; [2]University of Massachusetts Medical School, Worcester, MA*

TP 403 **MALDI Imaging Mass Spectrometry as a Tool to Evaluate Levels of ATP and its Metabolites in Mouse Tumor Models**; Stephanie Dale[1]; Cristine Quiason-Huynh[2]; *[1]Genentech, South San Francisco, CA; [2]Genentech, Inc., South San Francisco, CA*

TP 404 **Prospect of Using Small Molecules Based High-resolution DESI-QTOF-MS Imaging as a Direct Analysis Method of Classifying CNS Tumors in Diagnostics**; Lei Wang[1]; Xu Ma[1]; Chunyan Lan[1,2]; Hainan Li[3]; Linbo Cai[3]; Xiaofei Jia[4]; Huiqin Zhong[4]; *[1]National Center for Human Genetic Resources, National Research Institute for Health and Family Planning, Beijing, China; [2]Peking Union Medical College Graduate School, Beijing, China; [3]Guang Dong San Jiu Brain Hospital, Guangzhou, China; [4]Waters Technologies (Shanghai) Co, Ltd, Shanghai, China*

TP 405 **Visualization of the Distribution of Small Molecule in Pig-to-Nonhuman Primate Islet Xenotransplantation Model by MALDI-MRMS Imaging**; Jong Bok Seo[1]; Eui-Gil Jung[1]; Hee-Jung Kim[1]; Shin Kwon Kang[2]; JinNyoung Choi[2]; *[1]Korea Basic Science Institute, Seoul, South Korea; [2]Bruker Korea Co., Ltd, Seongnam-si, South Korea*

TP 406 **Imaging of Neurotransmitters Using AuNPs with Laser-Desorption Ionization Mass Spectrometry**; Nolan K McLaughlin[1]; Kate Stumpo[1]; *[1]University of Scranton, Scranton, PA*

TP 407 **Rearrangement of TMS and t-BDMS of Halogenated Saturated Aliphatic Alcohols in EI Mass Spectra**; Quan-long Pu[1]; Yufang Zheng[1]; Stephen stein[1]; *[1]NIST, Gaithersburg, MD*

IMAGING MS: SOFTWARE
408-415

TP 408 **Next-Generation Software for Visualization and Computational Analysis of High-performance Ion Mobility Molecular Imaging Data**; Lukasz Migas[1]; Jeffrey M. Spraggins[2,3]; Richard M. Caprioli[2,3]; Perdita E. Barran[4,5]; Raf Van de Plas[1,3]; *[1]Delft University of Technology, Delft, Netherlands; [2]Vanderbilt University, Nashville, TN; [3]Vanderbilt Mass Spectrometry Research Center and Department of Biochemistry, Nashville, TN; [4]University of Manchester, Manchester, United Kingdom; [5]Manchester Institute of Biotechnology, University of Manchester, United Kingdom*

TP 409 **Automatic Molecular Annotation of Mass Spectrometry Imaging Data**; Jan H. Kobarg[1]; Nikolas Kessler[2]; Wiebke Timm[2]; Janina Oetjen[2]; Klaus Steinhorst[1]; Stefan Schiffler[1]; Shannon Cornett[3]; Aiko Barsch[2]; Heiko Neuweger[2]; Alice Ly[2]; Dennis Trede[1]; *[1]SCiLS, Bremen, Germany; [2]Bruker Daltonik GmbH, Bremen, Germany; [3]Bruker Daltonics Inc., Billerica, MA*

TP 410 **Artificial Intelligence to Support Mass Spectrometry Imaging Analysis in Drug Discovery**; Ait-Belkacem Rima[1]; Fabien Pamelard[1]; Lauranne Poncelet[1]; Beuque Manon[1]; Gael Picard de Muller[1]; David Bonnel[1]; Jonathan Stauber[2]; *[1]Imabiotech, Loos, France; [2]ImaBiotech Corp, Boston, MA01821*

TP 411 **R/Python Application Programming Interface for MSI Statistical Analysis: Tumor Micro Environment Case Study**; Rima Ait-Belkacem[1]; Fabien Pamelard[1]; Gael Picard de Muller[1]; Lauranne Poncelet[1]; David Bonnel[1]; Jonathan Stauber[2]; *[1]Imabiotech, Loos, France; [2]ImaBiotech Corp, Boston, MA01821*

TP 412 **Reliable and Common Quantitative Color Scale to Evaluate at the Same Time Different Molecular Images in QMSI**; Rima Ait-Belkacem[1]; Fabien Pamelard[1]; Jordan Lerach[2]; Raphael Legouffe[1]; David Bonnel[1]; Jonathan Stauber[2]; *[1]Imabiotech, Loos, France; [2]ImaBiotech Corp, Boston, MA01821*

TP 413 **Longitudinal Quality Study of MSI PLatform for Pre-Clinical and Clinical Studies**; Rima Ait-Belkacem[1]; Fabien Pamelard[1]; Gael Picard de Muller[1]; Lauranne Poncelet[1]; David Bonnel[1]; Jonathan Stauber[2]; *[1]Imabiotech, Loos, France; [2]ImaBiotech Corp, Boston, MA01821*

TP 414 **A Proposed Software Method of Automatic Tissue Region Selection for Mass-Spectrometry Imaging Acquisition and Data Analysis**; Lei Wang[1]; Chunyan Lan[1,2]; Xu Ma[1]; *[1]National Center for Human Genetic Resources, National Research Institute for Health and Family Planning, Beijing, China; [2]Peking Union Medical College Graduate School, Beijing, China*

TP 415 **"Data Station One": An Open Source, Modular Platform for Custom Imaging Mass Spectrometer Systems**; Matthew Brantley[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX*

INFORMATICS: MULTIOMICS INTEGRATION
416-440

TP 416 **Mass-Spectrometry-Based Omics Technology to Reveal the Effect of Herbal Decoction in Cultured Osteoblasts**; Kwan Kin Leung[1]; Wong Tin Yan[2]; Yu Xiao Dan[1]; Leung Ka Wing[1]; Dong Tina Tingxia[1]; Lam Henry Hei Ning[2]; Tsim Karl Wah Keung[1]; *[1]Division of Life Science, Center for Chinese Medicine,Hong Kong university of science and technology, Sai Kung, China; [2]Department of Chemical & Biological Engineering,Hong Kong university of science and technology, Sai Kung, China*

TP 417 **LC-MS Based Multi-Omics Study on the Impact of Cysteine Feed on CHO Bioprocess mAb Titer, Specific Productivity and Product Quality**; Amr S Ali[1, 2]; Alan Gilbert[1]; Rashmi Kshirsagar[1]; Alexander R Ivanov[2]; Li Zang[1]; Barry L Karger[2]; *[1]Biogen, Cambridge, MA; [2]Northeastern University, Boston, MA*

TP 418 **Global High Resolution Mapping of Organellar Proteomic and Transcriptomic Correlation Profiles**; Mohamed A.W. Elzek[1]; Eneko Villanueva[1]; Tom S Smith[1]; Rayner Queiroz[1]; Kathryn Lilley[1]; *[1]University of Cambridge, Cambridge, United Kingdom*

TP 419 **MMCA: A Web-Based Server for Microbiome and Metabolome Correlation Analysis**; Yan Ni[1]; Mingming Su[2]; Yongqiong Deng[3]; Tianlu Chen[4]; Xiaojiao Zheng[4]; Wei Jia[5]; *[1]The Children's Hospital, Zhejiang University School of Medicine, Hangzhou, China; [2]Metabo-Profile biotechnology, Shanghai Co., Ltd., Shanghai, China; [3]Department of dermatology & STD, the Affiliated Hospital of Southwest Medical University, Luzhou, China; [4]Shanghai Jiao Tong University Affiliated Sixth People's Hospital, Shanghai, China; [5]University of hawaii Cancer Center, Honolulu, Hawaii*

TP 420 **Development of a Fast Open Source Proteogenomics Pipeline – ProteoAnnotator2**; Da Qi[1]; Andrew R. Jones[2]; Jeyan Thiyagalingam[2]; Fawaz Ghali[3]; *[1]BGI-Shenzhen, Shenzhen, China; [2]University of Liverpool, Liverpool, United Kingdom; [3]Manchester Metropolitan University, Manchester, United Kingdom*

TP 421 **Multi-omic Dissection of Oncogenically Active Epiproteomes Identifies Drivers of Invasive Breast Tumors**; John A Wrobel[1]; Ling Xie[1]; Li Wang[1]; Jian Jin[2]; Xian Chen[1]; *[1]University of North Carolina, Chapel Hill, NC; [2]Icahn School of Medicine at Mount Sinai, New York, NY*

TP 422 **PROTEOFORMER: Novel Developments in the Ribosome Profiling-Assisted Proteogenomic Hunt for New Proteoforms**; Steven Verbruggen[1]; Wim Van Criekinge[1]; Siegfried Gessulat[2]; Bernhard Kuster[2]; Mathias Wilhelm[2]; Petra Van Damme[3, 4]; Gerben Menschaert[1]; *[1]Ghent University, BioBix, Lab of Bioinformatics and Computational Genomics, Department of Mathematical Modelling, Statistics and Bioinformatics, Ghent, Belgium, Gent, Belgium; [2]Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; [3]Department of Biochemistry, Faculty of Health Sciences, Ghent University, Ghent, Belgium, Gent, Belgium; [4]VIB-UGent Center for Medical Biotechnology, Ghent, Belgium, Gent, Belgium*

TP 423 **A Mass Spectrometry Approach to Investigate the Role of EZH2 in Chromatin Remodeling, Cell Proliferation and Tumorigenesis**; Miranda L. Gardner[1]; Michael A. Freitas[1]; *[1]The Ohio State University, Columbus, OH*

TP 424 **Omni-MS: A Method for Concurrent LC-MS Analysis of Electrolytes, Small Molecules, Lipids, Proteins, Nucleic Acids, and Polysaccharides**; Austin Quach[1]; Brett Lomenick[1]; Alex J. Yoon[1]; Whitaker Cohn[1]; Julian P. Whitelegge[1]; Kym F. Faull[1]; *[1]University of California Los Angeles, Los Angeles, CA*

TP 425 **Phosphoproteomics Data Combined with Transcriptomics and Epigenomics Helps to Identify New Drug Targets against Methotrexate Resistance of Colon Cancer**; Alexander Kel[1]; Philip Stegmaier[1]; Olga Kel-Margoulis[1]; *[1]geneXplain GmbH, Wolfenbuettel, Germany*

TP 426 **Integrative Personalized Omics Profiling in Response to Acute Exercise in Healthy and Prediabetic Individuals**; Kevin Contrepois[1]; Kegan Moneghetti[2]; Si Wu[2]; Sara Ahadi[2]; Daniel Hornburg[2]; Eric Wey[2]; Ming-Shian Tsai[2]; Jeffrey W Christle[2]; Francois Haddad[2]; Michael Snyder[2]; *[1]Stanford University, Stanford; [2]Stanford University, Palo Alto, CA*

TP 427 **An Integrated Experimental and Computational Approach for the Characterization of Proteins of Unknown Function (PUFs) in *Clostridium thermocellum* DSM 1313**; Suresh Poudel[1]; Alex Cope[1, 2]; Kaela O'Dell[1, 3]; Adam M Guss[2]; Robert L. Hettich[2, 4]; *[1]University of Tennessee, Knoxville, TN; [2]Oak Ridge National Laboratory, Oak Ridge, TN; [3]Oak Ridge National Laboratory, Oak Ridge, Tennessee; [4]University of Tennessee, Knoxville, Knoxville, TN*

TP 428 **Conotoxin Exploitation from *Conus betulinus* Using an Integrated Approach of Transcriptomic and Peptidomics**; He yanbin[1]; Lin zhilong[1]; Luo Xing[1]; Ren zhe[1]; Roy Bhaskar[1]; Qi Da[1]; Liu Siqi[1]; *[1]BGI-Shenzhen, Shenzhen, China*

TP 429 **Meta-analysis of Public Proteomics Datasets Supports the Evaluation of Cancer Cell Lines as Tumour Models and Improves Drug Sensitivity Prediction**; Andrew F Jarnuczak[1]; Hanna Najgebauer[1]; Mitra P Barzine[1]; Deepti Jaiswal Kundu[1]; Fatemeh Zamanzad Ghavidel[2]; Yasset Perez-Riverol[1]; Irene Papatheodorou[1]; Alvis Brazma[1]; Juan Antonio Vizcaíno[1]; *[1]EMBL-EBI, Cambridge, United Kingdom; [2]University of Bergen, Bergen, Norway*

TP 430 **DeepRibo: Precise Gene Annotation of Prokaryotes Using Deep Learning and Ribosome Profiling Data, Validated with Mass Spectrometry Data**; Jim Clauwaert[1]; Gerben Menschaert[2]; Willem Waegeman[1]; *[1]KERMIT, Department of Data Analysis and Mathematical Modelling, Ghent University, Gent, Belgium; [2]BioBix, Lab of Bioinformatics and Computational Genomics, Department of Mathematical Modelling, Statistics and Bioinformatics, GENT, Belgium*

TP 431 **Proteogenomics Pipeline for Discovery of Genetically Variable Peptides in Humans**; Myles W. Gardner[1]; August E. Woerner[2]; Michael A. Freitas[3]; Nicolette C. Albright[1]; Alan R. Smith[1]; F. Curtis Hewitt[1]; *[1]Signature Science, LLC, Austin, TX; [2]Center for Human Identification, University of North Texas Health Science Center, Fort Worth, TX; [3]The Ohio State University, Columbus, OH*

TP 432 **A Multi-Omics Approach to Linking Proteomic Profiles and Metabolomic Phenotypes Provides Insight into Colorectal Cancer Cell Metabolism**; Peter Doubleday[1]; Ioanna Ntai[2]; Luca Fornelli[3]; Emily Boja[4]; Henry Rodriguez[4]; Neil L Kelleher[1]; *[1]Northwestern University, Evanston; [2]Thermo Fisher Scientific, San Jose, CA; [3]The University of Oklahoma, Norman, OK; [4]Office of Cancer Clinical Proteomics Research, NIH, Bethesda, MD*

TP 433 **Non-Ribosomal Peptide Antibiotic Discovery in Microbial Communities *via* Integration of Computational Metagenomics and Mass Spectrometry**; Bahar Behsaz[1]; Alexey Gurevich[2]; Rob Knight[3]; Pieter Dorrestein[1]; Pavel A. Pevzner[3]; Hosein Mohimani[4]; *[1]University of California San Diego, La Jolla, CA; [2]St. Petersburg State University, St. Petersburg, Russia; [3]University of California, San Diego, La Jolla, CA; [4]Carnegie Mellon University, Pittsburgh, PA*

TP 434 **Evaluating Machine Learning Methods Capable of Handling Missing Values for Protein Biomarker Studies**; David Nusinow[1]; John Szpyt[1]; Steven P Gygi[1]; *[1]Harvard Medical School, Boston, MA*



TP 435 **imetaQuantome Workflow: An Integrated Metaproteomics Workflow for Interactive, Statistical and Functional Microbiome Analysis**; Subina Mehta[1]; Ray Sajulga[1]; Caleb W Easterly[1]; Francesco Delogu[2]; Benoit J Kunath[2]; Praveen Kumar[1]; Marie Crane[3]; Emma Leith[1]; James E. Johnson[1]; Thomas McGowan[1]; Joel Rudney[1]; Phil B Pope[2]; Magnus Ø Arntzen[2]; Timothy J. Griffin[1]; Pratik D Jagtap[1]; *[1]University of Minnesota, Minneapolis, MN; [2]NMBU - Norwegian University of Life Sciences, Ås, Norway; [3]Macalester College, Saint Paul, MN*

TP 436 **Integration of Metabolomic and Lipidomic Workflows for Studying Clinical and Biological Systems**; Adriana Zardini Buzatto[1]; Shuang Zhao[1]; Ulrike Schweiger Hufnagel[2]; Aiko Barsch[2]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB; [2]Bruker Daltonik GmbH, Bremen, Germany*

TP 437 **pmartR: Software for Quality Control and Statistics Robust to Missing Data for Mass Spectrometry-Based Biological Data**; Lisa Bramer[1]; Kelly G. Stratton[1]; Bobbie-jo M. Webb-robertson[1]; Lee Ann McCue[1]; Bryan Stanfill[1]; Daniel Claborne[1]; Allison M. Thompson[1]; Iobani Godinez[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

TP 438 **Metaproteomics Powered By Metatranscriptomics:Towards a Multi-Omic Functional Microbiome Analysis**; Pratik Dilip Jagtap[1]; Praveen Kumar[1]; Francesco Delogu[2]; Benoit J Kunath[2]; Sujun Li[3]; Marie Crane[4]; Subina Mehta[1]; Ray Sajulga[1]; Emma Leith[1]; James E. Johnson[5]; Yuzhen Ye[3]; Berenice Batut[6]; Haixu Tang[3]; Phil B Pope[2]; Magnus Ø Arntzen[2]; Timothy Griffin[1]; *[1]University of Minnesota, Minneapolis, MN; [2]Faculty of Chemistry, Biotechnology and Food Science, NMBU, As, Norway; [3]School of Informatics, Computing, and Engineering, Indiana University,, Bloomington, IN; [4]Macalester College, Saint Paul, MN; [5]Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, MN; [6]Bioinformatics Group, University of Freiburg, Freiburg, Germany*

TP 439 **Integrated Omics Analysis Across 32 Human Tissues**; Lihua Jiang[1]; Meng Wang[2]; Shin Lin[3]; Ruiqi Jian[2]; Joanne Chan[2]; Xiao Li[2]; Huaying Fang[2]; Hua Tang[2]; Michael Snyder[2]; *[1]Stanford University, Stanford, CA; [2]Stanford University, Palo Alto, CA; [3]University of Washington, Seattle, WA*

TP 440 **SysMet: A Tool for Integrative Systems Metabolomics**; Mohammad R Nezami Ranjbar[1]; Ziling Fan[1]; Yan Gao[1]; Habtom W Ressom[1]; *[1]OmicsCraft LLC, Washington, DC*

INSTRUMENTATION: MINI/PORTABLE/FIELDABLE MS 441-457

TP 441 **A Mini Quadrupole Mass Spectrometer with a Continuous Atmospheric Pressure Interface**; Ranran Liu; *Institute of Atmospheric Physics, Chinese Academy of Sciences, Beijing, China*

TP 442 **MOMA Mass Spectrometer Laser Desorption Ionization Investigation of Spiked Mineral Samples for ExoMars Mission Planning**; Friso h.w. Van amerom[1]; Marco Castillo[2]; Xiang Li[2]; Ryan Danell[3]; Desmond Kaplan[4]; Eric I. Lyness[5]; Stephanie A. Getty[6]; Andrej Grubisic[6]; William B. Brinckerhoff[6]; Paul R. Mahaffy[6]; *[1]Mini-Mass Consulting, Inc, Hyattsville, MD; [2]University of Maryland, Baltimore, MD; [3]Danell Consulting, Inc., Winterville, NC; [4]Kapscience, LLC, Tewksbury, MA; [5]Microtel-LLC, Greenbelt, MD; [6]NASA Goddard Space Flight Center, Greenbelt, MD*

TP 443 **Development of the Advanced Resolution Organic Molecular Analyzer (AROMA)**; Adrian Southard[1]; Emanuel Hernandez[2]; Ryan Danell[3]; Cynthia Gundersen[4]; Lars Hovmand[5]; Andrej Grubisic[2]; Ricardo Arevalo[6]; *[1]Universities Space Research Association, Greenbelt, MD; [2]NASA Goddard Space Flight Center, Greenbelt, MD; [3]Danell Consulting, Inc., Winterville, NC; [4]ADNET System, Inc., Bethesda, MD; [5]Linear labs, Washington, DC; [6]University of Maryland, College Park, MD*

TP 444 **Calibration Drift and Maintaining Requirements in Harsh Environmental Conditions with the Mars Organic Molecule Analyzer (MOMA) Mass Spectrometer**; Ryan M. Danell[1]; Andrej Grubisic[2]; Veronica Pinnick[2]; Desmond A. Kaplan[3]; Friso Van Amerom[4]; Stephanie A. Getty[2]; William B. Brinckerhoff[2]; *[1]Danell Consulting, Inc., Winterville, NC; [2]NASA Goddard Space Flight Center, Greenbelt, MD; [3]KapScience LLC, Tewksbury, MA; [4]Mini-Mass Consulting, Inc, Hyattsville, MD*

TP 445 **A Handheld Mass Spectrometer for In-Field and POC Analysis**; Bin Jiao[1]; Xinwei Liu[1]; Jiexun Bu[2]; Ningxi Li[1]; Zheng Ouyang[1]; *[1]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China; [2]PURSPEC Technologies Inc., Beijing, China*

TP 446 **Development of a Miniature GC-MS Instrument for Fieldable Applications**; Vladimir M. Doroshenko[1]; Victor Laiko[1]; Eugene Moskovets[1]; Konstantin Novoselov[1]; Tzu-Hsuan Chang[2]; Daniel Struk[2]; Jean-Marie D. Dimandja[2]; Milad Navaei[2]; Peter J. Hesketh[2]; *[1]MassTech, Inc., Columbia, MD; [2]Georgia Institute of Technology, Atlanta, GA*

TP 447 **3D Real Time Monitoring of Unintended Concentration of H2/Air in FCV Applications**; Takashi Nohmi[1, 2]; Toshio Mogi[2]; *[1]HysafeNohmi, Setagaya-Ku, Japan; [2]The University of Tokyo, Bunkyo, Japan*

TP 448 **The Development of Miniature MALDI Digital Ion Trap Mass Spectrometer**; Kosuke Hosoi[1]; Masaji Furuta[1]; Hideharu Shichi[1]; Shosei Yamauchi[1]; Kiyoshi Watanabe[1]; Makoto Hazama[1]; Kei Kodera[1]; Shinichi Iwamoto[1]; Koichi Tanaka[1]; *[1]Shimadzu Corporation, Kyoto, Japan*

TP 449 **The Effects of Electrode Misalignment on the Performance of a Linear Wire Ion Trap**; Radhya W. Gamage[1]; Daniel E. Austin[1]; *[1]Brigham Young University, Provo, UT*

TP 450 **Profiling Agrochemical Residues in Produce *via* Paper Cone Spray Ionization and Portable Instrumentation**; Alyssa J. Gasa[1]; Makoy R. Overfelt[1]; Christopher Mulligan[2]; *[1]Illinois state university, Normal, IL; [2]Illinois State University, Normal, IL*

TP 451 **Method to Improve the Higher Pressure Operation Characteristics of Microchannel Plate Detectors, and Its Effect on Performance of Miniature MS**; Masahiro Hayashi; *Hamamatsu Photonics K.K., Iwata, Japan*

TP 452 **Microscale Linear Ion Trap Mass Spectrometer**; Trevor Decker[1]; Yajun Zheng[2]; Aaron Ruben[1]; Xiao Wang[3]; Stephen Lammert[3]; Aaron Hawkins[1]; Daniel Austin[1]; *[1]Brigham Young University, Provo, UT; [2]Xi'an Shiyou University, Xi'an, China; [3]PerkinElmer Health Sciences Inc., American Fork, UT*

TP 453 **Development of a Flexible GC Transfer Line for a Field-Deployable GC-EI/MS**; Steffen Bräkling[1]; Kai Kroll[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

TP 454 **Development of Micro-Time-of-Flight Mass Spectrometer for *in situ* Gas Analysis**; Alex Sonnette[1]; Frederic Progent[2]; Jerome Tupinier[2]; Pierre-Etienne Buthier[2]; Jean-Christophe Lictevout[2]; Sébastien Vigne[2]; Thomas Alava[3]; *[1]CEA, Arpajon, France; [2]CEA, Arpajon, France; [3]CEA, Grenoble, France*

TP 455 **A Mixed Computational Fluid Dynamics and Direct Simulation Monte Carlo model of the Intermediate Pressure Regions of a Miniature ESI-MS**; Edward Crichton[1]; Rantej S Kler[1]; Richard W Moseley[1]; *[1]Microsaic Systems, Woking, United Kingdom*

TP 456 **Evaluation of a Portable GC-MS Equipped with a Planar-LTM Column for Chemical and Riot Control Agent Screening Applications**; Zachary E Lawton[1]; Thomas Saul[2]; Evan Dumal[3]; Sara Paalhar[3]; Becky Stilley[3]; Nathan

Doll[3]; [1]PerkinElmer, Shelton, CT; [2]Smiths Detection, Edgewood, MD; [3]MRIGlobal, Kansas City, MO

TP 457 **Fieldable Atmospheric Pressure Ion Mobility Linear Ion Trap Mass Spectrometer for On-site Chemical Identification**; Greg Brabeck[1]; Mark Osgood[1]; Tomás F Gutierrez[1]; Eugenie Hainsworth[1]; Marina Loginowski[1]; Ching Wu[1]; [1]Excellims Corporation, Acton, Massachusetts

INSTRUMENTATION: NEW DEVELOPMENTS IN ION DETECTION
458-496

TP 458 **Development of MCP+AD Detector for Q-TOF Called MIGHTION with a Large 42 mm Effective Area and Bipolar Ion Detection**; Hiroshi Kobayashi[1]; Sayaka Takatsuka[1]; [1]HAMAMATSU PHOTONICS K.K., Iwata, Japan

TP 459 **Development of Lead-Free Channel Electron Multiplier Named CERARION that Achieves Over 100 uA DC Output**; Takeshi Endo[1]; Hiroshi Kobayashi[1]; Kengo Watase[1]; hayato inoue[1]; [1]HAMAMATSU PHOTONICS K.K., Iwata, Japan

TP 460 **Peak Amplitude vs. Peak Area: Which Better Measures Charge in CDMS?**; Jiuzhi Gao[1]; Daniel E. Austin[1]; [1]Brigham Young University, Provo, UT

TP 461 **Deconvolution of Complex Protein Mixtures Using Orbitrap-Based Charge Detection Mass Spectrometry**; Jared O. Kafader[1]; Rafael D. Melani[1]; Bryan P. Early[1]; Kenneth R. Durbin[1]; Benjamin Soye[1]; Mike W. Senko[2]; Vlad Zambouskov[2]; Alexander A Makarov[3]; Joshua T. Maze[4]; Deven L. Shinholt[4]; Steven Beu[5]; Neil L Kelleher[1]; Philip D. Compton[1]; [1]Northwestern University, Evanston, IL; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Bremen, Germany; [4]Thermo Fisher Scientific, Austin, TX; [5]S.C. Beu Consulting, Austin, TX

TP 462 **Development of an α-particle and TOF Ion Detector for Precise Measurements of Atomic Mass of Superheavy Nuclei**; Toby Shanley[1]; Wayne Sheils[1]; Michiharu Wada[2]; Toshitaka Niwase[2,3]; Yair Benari[1]; Hermann Wollnik[4]; Peter Schury[2]; [1]ETP Ion Detect, Sydney, Australia; [2]KEK, High Energy Research Accelerator Organisation, Hirasawa, Japan; [3]Kyushu University, Fukuoka, Japan; [4]New Mexico State University, Las Cruces, NM

TP 463 **Sub-Nanosecond, Stable and Long-Lifetime Detector for TOF Applications**; Jonathan Garel[1]; Semyon Shofman[1]; Amit Weingarten[1]; Sasha kadyshevitch[1]; Eli Cheifetz[1]; [1]El-Mul Technologies, Rehovot, Israel

TP 464 **Negative Electron Affinity Material for Increased Ion Detection Sensitivity in Electron Multipliers**; Toby Shanley[1]; Wayne Sheils[1]; [1]ETP Ion Detect, Sydney, Australia

TP 465 **Paper Spray Ionization Mass Spectrometry of Sebum Samples: A Step Towards Rapid, Early Diagnosis of Parkinson's Disease**; Depanjan Sarkar[1]; Drupad Trivedi[1]; Caitlin Walton-Doyle[1]; Joy Milne[1]; Eleanor Sinclair[1]; Monty Silverdale[1]; Perdita Barran[1]; [1]University of Manchester, Manchester, United Kingdom

TP 466 **Charge-Sensing Particle Detector (CSPD): A Sensitivity-Enhanced Faraday Cup**; Szu-Wei Chou[1]; Yi-Kun Lee[2]; Yi-Teng Hsiao[2]; Liang-Chun Fan[2]; Chun-Yen Cheng[2]; [1]AcroMass technologies, Inc., Taipei, Taiwan; [2]AcroMass Technologies, Inc., Hsinchu, Taiwan

TP 467 **Enhanced Charge Detection Mass Spectrometry Precision with a Low-Noise Amplifier Without a Feedback Resistor**; Aaron R Todd[1]; Andrew W Alexander[1]; Martin F Jarrold[1]; [1]Indiana University, Bloomington, IN

TP 468 **Tantalum-Based Superconducting Tunnel Junction Cryodetection Mass Spectrometry**; Logan Plath[1]; Mohammad A. Halim[1]; Stephan Friedrich[2]; Francisco Ponce[3]; Jack Harris[4]; Robin Cantor[5]; Mark E. Bier[1]; [1]Carnegie Mellon University, Pittsburgh, PA; [2]Lawrence Livermore National Laboratory, Livermore, CA; [3]Stanford University, Palo Alto, CA; [4]XIA LLC, Hayward, CA; [5]STAR Cryoelectronics, Santa Fe, NM

TP 469 **Atomic Layer Coating Enabled Performance Improvements of Channel Electron Multipliers (CEM)**; Matthew Breuer[1]; Paula Holmes, Dr. [1]; [1]Photonis USA, Sturbridge, MA

TP 470 **Multiplexing in Charge Detection Mass Spectrometry: Rapid Measurement of Large Native Proteins and Macromolecular Complexes**; Conner C Harper[1]; Andrew G. Elliott[1]; Evan R. Williams[1]; [1]University of California, Berkeley, Berkeley, CA

TP 471 **Generation of Electrosprayed Ions for Fundamental Studies Using a Linear Ion Trap Coupled to a Superconducting Tunnel Junction Cryodetector**; Mohammad Abdul Halim[1]; Logan Plath[1]; Jonathan Shulgach[1]; Mark E. Bier[1]; [1]Carnegie Mellon University, Pittsburgh, PA

TP 472 **Distance-of-Flight Mass Spectrometry Using a Semiconductor Ion Detector Array**; Steven Ray; University at Buffalo, SUNY, Buffalo, NY

TP 473 **High-Pressure Solid-State Ion Detector with 10-uV/e- Gain and 180-e- Noise**; Yixin Song[1]; Justin Chu[1]; Joan Magalhaes[1]; Jacob Nowjack[1]; Jace Rozsa[1]; Eric Swindlehurst[1]; Sanjiv Pant[1]; Kent Layton[1,2]; Steve Lammert[3]; Xiao Wang[3]; Edgar Lee[3]; Nathan Porter[3]; Milton Lee[1]; Aaron Hawkins[1]; Shiuh-hua Wood Chiang[1]; [1]Brigham Young University, Provo, UT; [2]ON Semiconductor, Lindon, UT; [3]PerkinElmer Health Sciences Inc., American Fork, UT

TP 474 **Electron Ionization LC-MS with Supersonic Molecular Beams - Drug Impurities Analysis and Combination with GC-MS in One System**; Svetlana Tsizin[1]; Tal Alon[1]; Alexander B. Fialkov[1]; Aviv Amirav[1]; [1]Tel-Aviv University, Tel-Aviv, Israel

TP 475 **The Use of a Cooled Inlet System to Enable the Measurement of Negatively Charged Compounds Using CIMS**; Alan T. Taylor[1]; C. Logan Mackay[1]; M. J. Cowley[1]; N. McKeown[1]; [1]University of Edinburgh, Edinburgh, United Kingdom

TP 476 **Development of a GC-APCI Interface for an Orbitrap MS**; Joshua B Powers[1]; Shawn R Campagna[1]; [1]University of Tennessee, Knoxville, TN

TP 477 **Mechanospray Ionization (MSI) of Macromolecules Produces Lower Average Charge States and Lower Internal Energy Ions than ESI**; Liam Dugan[1]; Mark E. Bier[1]; [1]Carnegie Mellon University, Pittsburgh, PA

TP 478 **Combined Atomic and Molecular (CAM) Ionization Source with an Orbitrap 1M: Elemental, Isotopic, and Molecular MS at Resolution of >1.5M**; R. Kenneth Marcus[1]; Edward D Hoegg[2]; David W Koppenaal[2]; Joanna Szpunar[3]; Simon Godin[3]; Ryszard Lobinski[3]; [1]Clemson University, Clemson, SC; [2]Pacific Northwest National Laboratory, Richland, WA; [3]CNRS, InInstitute of Analytical Sciences and Physical Chemistry for the Environment and Materials, Pau, France

TP 479 **Liquid Sampling – Atmospheric Pressure Glow Discharge (LS-APGD) Interfaced with a Compact (Quadrupole) Mass Spectrometer for Analysis of Diverse Samples**; Tyler Williams[1]; R. Kenneth Marcus[1]; [1]Clemson University, Clemson, SC

TP 480 **Direct Analysis of Contaminants in Soil, Aqueous, and Biological Samples Using Membrane Introduction Tandem Mass Spectrometry with Liquid Electron Ionization**; Gregory W. Vandergrift[1,2]; Joseph Monaghan[1]; Erik T. Krogh[1,2]; Christopher G. Gill[1,2,3,4]; [1]Appl. Env. Res. Labs. (AERL), Vancouver Island University, Chemistry Department, Nanaimo, BC; [2]University of Victoria, Chemistry Department, Victoria, BC; [3]Simon Fraser University, Chemistry Department, Burnaby, BC; [4]University of Wasington, DEOHS, Seattle, WA

TP 481 **Single-Cell Analysis by Mass Spectrometry Using Electro-Migration and Electroporation**; Zishuai Li[1]; Zhengmao Wang[2,3]; Xiaoxiao Ma[4]; Junmin Pan[2,3]; Zheng Ouyang[4,5]; *[1]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China; [2]Laboratory for Marine Biology and Biotechnology, Qingdao National Laboratory for Marine Science and Technology, Qingdao, China; [3]MOE Key Laboratory of Protein Sciences, Tsinghua-Peking Center for Life Sciences, School of Life Sciences, Tsinghua University, Beijing, China; [4]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instruments, Tsinghua University, Beijing, China; [5]Weldon School of Biomedical Engineering, Purdue University, West Lafayette, ILLINOIS*

TP 482 **Microfluidic Open Interface with Liquid Electron Ionization Mass Spectrometry: Rapid Measurement of THC and Other Cannabinoids in Different Matrices**; Pierangela Palma[1]; Veronica Termopoli[1]; Giorgio Famiglini[1]; Greta Giacomelli[1]; Achille Cappiello[1]; Emir Nazdrajić[2]; Janusz Pawliszyn[2]; *[1]University of Urbino, Urbino, Italy; [2]University of Waterloo, Waterloo, ON*

TP 483 **Static Membrane Extraction Mass Spectrometry for Space Applications**; R. Timothy Short[1]; Strawn K. Toler[1]; Jennifer C. Stern[2]; Charles A. Malespin[2]; Brian M. Leiter[3]; *[1]SRI International, St Petersburg, FL; [2]NASA Goddard Space Flight Center, Greenbelt, MD; [3]ADNET System, Inc., Bethesda, MD*

TP 484 **Simulation of Isotherm HiKE-IMS – MS Transfer Stage**; Robin Hillen[1]; Walter Wissdorf[1]; Maria Allers[2]; Hendrik Kersten[1]; Stefan Zimmermann[2]; Thorsten Benter[1]; *[1]Bergische Universität Wuppertal, Wuppertal, Germany; [2]Leibniz Universität Hannover, Hannover, Germany*

TP 485 **Microflow LC-Nanospray ESI-MS**; Daojing Wang[1]; Pan Mao[1]; Yuchao Chen[1]; *[1]Newomics Inc., Berkeley, CA*

TP 486 **A Novel Method for NH4+ Reagent Ion Production in PTR-MS and its Applications**; Christian Lindinger[1]; Eugen Hartungen[1]; Rene Gutmann[1]; Alfons Jordan[1]; Lukas Märk[1]; Philipp Sulzer[1]; *[1]IONICON Analytik GmbH., Innsbruck, Austria*

TP 487 **Optimized Nanoflow ESI Source to Eliminate the Need for Tuning**; Yang Kang[1]; Bradley B. Schneider[1]; Leigh Bedford[1]; Thomas R. Covey[1]; *[1]SCIEX, Concord, ON*

TP 488 **High-Throughput, Low-Cost Reaction Screening Apparatus Using a Modified 3D Printer**; Robert Schrader[1]; Stephen T Ayrton[1]; R. Graham Cooks[1]; *[1]Purdue University, West Lafayette, IN*

TP 489 **Development of a Novel Tantalum Cathode for Determing Trace Elements in Soils by Glow Discharge Mass Spectrometry**; Rong Qian[1]; Shangjun Zhuo[1]; Jiangli Dong[1]; *[1]Shanghai Institute of Ceramics, Chinese Academy of Sciences, Shanghai, China*

TP 490 **Efficient Ionization of Challenging Pesticides Using Liquid Chromatography/Mass Spectrometry and Dielectric Barrier Discharge Ionization (DBDI)**; Juan F Garcia-Reyes[1]; Julio César Benítez-Villalba[2]; Miriam Beneito-Cambra[1]; Bienvenida Gilbert-López[1]; Antonio Molina-Díaz[1]; Sebastian Brandt[3]; Joachim Franzke[3]; *[1]University of Jaen, Jaen, Spain; [2]Universidad Nacional de Asuncion, Facultad de Ciencias Exactas y Naturales, San Lorenzo, Paraguay; [3]Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany*

TP 491 **Microsampling with Cotton Threads and Direct Analysis *via* Ambient Mass Spectrometry**; Devin Swiner[1]; Sierra Jackson[1]; George R. Durisek[1]; Bridget K. Walsh[1]; Yaman Kouatli[1]; Abraham K. Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH*

TP 492 **Characterization and Development of a Reagent Cation Source for NETD**; Steven J Kregel[1]; Benton J Anderson[2]; Michael S Westphall[1]; Joshua J Coon[1,2,3,4]; *[1]Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI; [2]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [3]Morgridge Institute for Research, Madison, WI; [4]Genome Center of Wisconsin, Madison, WI*

TP 493 **Resolving Elemental Isobaric Interferences with the Liquid Sampling-Atmospheric Pressure Glow Discharge / Orbitrap System for High Precision Isotope Ratio Measurements**; Edward D Hoegg[1,2]; David W Koppenaal[2]; Simon Godin[3]; Joanna Szpunar[3]; Ryszard Lobinski[3]; R. Kenneth Marcus[1]; *[1]Clemson University, Clemson, SC; [2]Pacific Northwest National Laboratory, Richland, WA; [3]CNRS, InInstitute of Analytical Sciences and Physical Chemistry for the Environment and Materials, Pau, France*

TP 494 **An Integrated Electrocatalytic nESI-MS Platform for Direct Analysis of C=C Isomers in Fatty Acids Derived from Complex Biofluids**; Kavyasree Chintalapudi[1]; Abraham K. Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH*

TP 495 **Quantitative Analysis of Anticancer Drugs in Live Single Suspension Cells: From Cell Lines to Patient Samples**; Shawna Standke[1]; Ryan Bensen[1]; Devon Colby[1]; Anh Le[1]; Naga Rama Kothapalli[1]; Jonathan E. E. Heinlen[2]; Anthony Burgett[1]; Zhibo Yang[1]; *[1]University of Oklahoma, Norman, OK; [2]University of Oklahoma, Health and Science Center, Oklahoma City, OK*

TP 496 **Direct Analysis of Complex Mixtures by Non-contact Nano-Electrospray Mass Spectrometry Coupled with Simultaneous Atmospheric Pressure Chemical Ionization**; Dmytro S Kulyk[1]; Abraham K. Badu-Tawiah[1]; *[1]OSU, Columbus, OH*

ION MOBILITY: APPLICATIONS I
497-519

TP 497 **Probing the Conformational Adaptations of Thermoresponsive Polymers by Ion-Mobility Mass Spectrometry**; Savannah Snyder[1]; Megan A Cruz[2]; Abraham Joy[2]; Chrys Wesdemiotis[1]; *[1]The University of Akron Chemistry Department, Akron, OH; [2]The University of Akron, Akron*

TP 498 **Ergodic and Non-Ergodic Mobility Selected Fragmentation of Isomeric Model Peptides**; Noa deHaseth[1]; Jacob Porter[2]; Francisco Fernandez-Lima[2]; *[1]University of Florida, Gainesville, FL; [2]Florida International University, Miami, FL*

TP 499 **Demonstration of the Unique Capabilities of Cyclic Ion Mobility High Resolution Mass Spectrometry to Resolve Stereoisomeric and Regioisomeric Saponin Ions**; Emmanuel Colson[1]; Corentin Decroo[1]; Julien De Winter[1]; Dale Cooper-Shepherd[2]; Martin Palmer[2]; Jan Claereboudt[2]; Pascal Gerbaux[1]; *[1]University of Mons, Mons, Belgium; [2]Waters Corportaion, Cheshire, United Kingdom*

TP 500 **Comparing Solution Phase and Gas Phase Protein Stability Using Collisional Induced Unfolding**; Lucienne Nouchikian[1,2]; Derek J Wilson[1,2]; *[1]York University, Toronto, ON; [2]Center for Research in Mass Spectrometry, Toronto, Ontario*

TP 501 **Analysis of Specific Metal Binding to Alpha-Synuclein with Collisional Induced Unfolding**; Neil R. Quebbemann[1]; Joseph A. Loo[1]; *[1]University of California Los Angeles, Los Angeles, CA*

TP 502 **Utilization of Enhanced Shape Selective Information Obtained from a Cyclic Ion Mobility-Enabled –Mass Spectrometer for the Characterisation of Complex Mixtures**; Javeria Mehboob[1]; James Scrivens[1]; Gillian Taylor[1]; Safwan Akram[1]; Martin Palmer[2]; Jakub Ujma[2]; Kevin Giles[2]; Jonathan P Williams[2]; David Portwood[3]; Pablo Navarro[3]; *[1]Teesside University, Middlesbrough, United Kingdom; [2]Waters Corportaion, Cheshire, United Kingdom; [3]Syngenta Jealott's Hill International Research Centre, Bracknell, United Kingdom*

TP 503 **Pursuit of Bottom-Up, Middle-Down, and Top-Down Glycoconjugate Analysis Enabled Through Online CE-ESI-IMS**; Daniel Delafield[1]; Gongyu Li[2]; Lingjun Li[3]; *[1]University of Wisconsin Madison, Madison, WI; [2]University of Wisconsin - Madison, Madison, WI; [3]University of Wisconsin, Madison, Madison, WI*

TP 504 **Following Conformational Changes in Knot Proteins with nESI-TIMS-MS: Solution vs Gas Phase**; Jean R. N. Haler[1]; Kevin Jeanne Dit Fouque[1]; Juan Camilo Molano-Arevalo[1]; Fenfei Leng[1]; Francisco A. Fernandez-Lima[1]; *[1]Florida International University, Miami, FL*

TP 505 **An Investigation into the use of Cyclic Ion Mobility for the Separation of Biopharmaceutical Peptide and Protein Modifications**; Jim Langridge[1]; Henry Shion[2]; Martin Palmer[3]; Weibin chen[2]; Dale A Cooper-Shepherd[3]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters Corporation, Milford, MA; [3]Waters Corporation, Wilmslow, United Kingdom*

TP 506 **Fast Collision Induced Unfolding Coupled to Droplet Microfluidic-Based Sample Introduction for High-Throughput Protein Structural Analysis and Drug Discovery**; Cara I. D'Amico[1]; Daniel A. Polasky[1]; Sugyan M. Dixit[1]; Robert T. Kennedy[1]; Brandon T. Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI*

TP 507 **Structural Characterization of Carbohydrates Oligosaccharide using Tandem Trapped Ion Mobility Spectrometry–Mass Spectrometry**; Jusung Lee[1]; Christian Bleiholder[1]; *[1]Florida State University, Tallahassee, FL*

TP 508 **Direct Identification of Endogenous Ligands Bound to Specific Protein Conformations Using Multistage Gas Phase Separation on a Cyclic-Mobility Mass Spectrometer**; Idlir Liko[1]; Joseph F Gault[2]; Martin Palmer[3]; Dale A Cooper-Shepherd[3]; Jakub Ujma[3]; Carol V. Robinson[2]; *[1]OMass Therapeutics, Oxford, United Kingdom; [2]Oxford University, Oxford, United Kingdom; [3]Waters Corporation, Wilmslow, United Kingdom*

TP 509 **Analysis of Lipid Signaling Class Analytes Using a Travelling Wave Cyclic Ion Mobility Separator**; Mike McCullagh[1]; Martin Palmer[1]; Emma Marsden-Edwards[1]; James I Langridge[1]; Johannes PC Vissers[1]; *[1]Waters Corporation, Wilmslow, United Kingdom*

TP 510 **Separation of Asp/IsoAsp Isobaric Peptides Using Trapped Ion Mobility Spectrometry (TIMS)**; Anjali Alving[1]; Shourjo Ghose[1]; Leah (Hanliu) Wang[2]; Olga Friese[2]; *[1]Bruker Scientific, Billerica, MA; [2]Pfizer, Chesterfield, MO*

TP 511 **Fast Identification and Simultaneous Separation of Electrochemically Generated Isomeric Xenobiotic Phase-I Metabolites by means of Trapped Ion Mobility-Mass Spectrometry**; Jens Fangmeyer[1]; Simon Gereon Scheeren[1]; Robin Schmid[1]; Uwe Karst[1]; *[1]University of Muenster, Institute of Inorganic and Analytical Chemistry, Muenster, Germany*

TP 512 **All Ion Unfolding/Fragmentation (AIU/AIF): A Modified Native Ion Mobility–Mass Spectrometry (IM-MS) Approach for Diagnostic Glycoprotein Analysis**; Ashley Phetsanthad[1]; Gongyu Li[2]; Lingjun Li[1,2]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI*

TP 513 **The Performance of a New Ion Mobility Spectrometer Designed to Measure Singly-charged Protein Ions**; W Henry Benner[1]; Ben Aguilar[1]; *[1]Ion Dx, Monterey, CA*

TP 514 **Short nanoLC Gradients Optimize Throughput on a tims Equipped QTOF for Deep Proteome Measurements**; Thomas Kosinski[1]; Scarlet Koch[1]; Thorsten Lederthell[1]; Christian Meier-Credo[1]; Christoph Gebhardt[1]; Gary Kruppa[2]; Heiner Koch[1]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Bruker Daltonics Inc., Billerica, MA*

TP 515 **A Non Targeted Approach to the Development of a Food Additive CCS Screening Library and its Application**; Mike McCullagh[1]; Mike Wilson[1]; Severine Goscinny[2]; Kenneth Rosnack[3]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Sciensano, Brussels, Belgium; [3]Waters Corporation, Milford, MA*

TP 516 **Investigations into Cross-Platform and Long-Term Robustness of a CCS Metric**; David Douce[1]; Mike McCullagh[2]; Michelle Wood[2]; Nayan Mistry[2]; Severine Goscinny[3]; Petur Dalsgaard[4]; *[1]Waters (MS Technologies), Wilmslow, United Kingdom; [2]Waters Corporation, Wilmslow, United Kingdom; [3]Sciensano, 14, rue Juliette Wytsman,, Belgium; [4]Department of Forensic Medicine, University of Copenhagen,, Copenhagen, Denmark*

TP 517 **Effects of Osmolytes on Conformations of Model Proteins as Studied by IM-MS**; Christopher Mallis[1]; David H. Russell[1]; *[1]Texas A&M University, College Station, TX*

TP 518 **Ion Mobility-Accelerated Peptide Separation in Time and Space to Unveil Human Proteomes**; Yasushi Ishihama[1]; Kosuke Ogata[1]; Ryo Kajita[2]; Heiner Koch[3]; Koshi Imami[1]; Naoyuki Sugiyama[1]; *[1]Kyoto University, Kyoto, Japan; [2]Bruker Japan K.K., Yokohama, Japan; [3]Bruker Daltonik GmbH, Bremen, Germany*

TP 519 **"Zero Charge Selection" Ion Mobility-Mass Spectrometry Reveals the Effect of Sialylation on Glycoprotein Structures**; Gongyu Li[1]; Lingjun Li[2]; *[1]University of Wisconsin-Madison, Madison, WI; [2]University of Wisconsin, Madison, Madison, WI*

ION MOBILITY: FAIMS/DMS
520-529

TP 520 **Simplifying uranium isotope ratio (IR) analysis with nanospray differential mobility spectrometry- mass spectrometry (DMS-MS)**; Ifeoluwa Ayodeji[1]; Theresa Evans-Nguyen[2]; *[1]University of South Florida, Tampa, FL; [2]University of Florida, Tampa, FL*

TP 521 **Chemical Kinetics and Ion Transport Simulations: Cluster Dynamics in Differential Ion Mobility Spectrometry**; Walter Wissdorf[1]; Duygu Erdogdu[1]; Florian Stappert[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

TP 522 **Validated FIA-FAIMS SRM MS Approaches for Vicine and Convicine Quantification from Faba Beans and Implications for Molecular Marker Analysis**; Haixia Zhang[1]; Randall W Purves[1]; Rob Stonehouse[1]; Pete M. P. Iannetta[2]; Jodi Souter[3]; Thomas D. Warkentin[1]; Albert Vandenberg[1]; *[1]University of Saskatchewan, Saskatoon, SK; [2]The James Hutton Institute, Dundee, United Kingdom; [3]Hemp Genetics International, Saskatoon, SK*

TP 523 **FAIMS Separation of Fentanyl-Related Compounds Using Vapor Modification**; Nathan a Grimes[1]; Ifeoluwa Ayodeji[2]; Theresa Evans-Nguyen[1]; *[1]University of South Florida, Tampa; [2]University of South Florida, Tampa, FL*

TP 524 **LC-ultra FAIMS-MS Separation of Opioid Isomers Using Solvent Vapor Addition**; Kevin Davis[1]; Michael Wei[1]; Robin H.J. Kemperman[1]; Timothy J. Garrett[2]; Richard A Yost[1]; *[1]Department of Chemistry, University of Florida, Gainesville, FL; [2]Department of Pathology, Immunology, and Laboratory Medicine, University of Florida, Gainesville, FL*

TP 525 **Affecting FAIMS Separation with Trace Levels of Gas Modifiers**; Michael Belford[1]; Michael Wei[2]; Eloy R. Wouters[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]University of Florida, Gainesville, FL*

TP 526 **Developing the Research to Routine Workflows with FAIMS: Automating Large-Scale SRM Method Creation for Routine Plasma Proteomics Screening**; Scott Peterman[1]; Kerry Hassell[2]; Mary L. Blackburn[3]; Romain Huguet[3]; Michael Volny[3]; Michael Belford[3]; Satendra Prasad[3]; *[1]Thermo Fisher Scientific, Grimes, IA; [2]Thermo*

Fisher Scientific, Somerset, NJ; [3]Thermo Fisher Scientific, San Jose, CA 95134

TP 527 **FAIMS Pro™ Interface Coupled to Triple Quadrupole Mass Spectrometry for Quantification of Peptides in Complex Matrices**; Michael Volny[1]; Claudia P.B. Martins[1]; Mary L. Blackburn[1]; Michael W. Belford[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

TP 528 **– Lifting the Albumin Curtain to Increase Plasma Proteome Profiling: Incorporating Differential Ion Mobility for Increased Protein Coverage**; Scott Peterman[1]; Romain Huguet[2]; Michael Belford[2]; Satendra Prasad[2]; Susan E. Abbatiello[3]; *[1]Thermo Fisher Scientific, Grimes, IA; [2]Thermo Fisher Scientific, San Jose, CA 95134; [3]Northeastern University, Boston, MA*

TP 529 **Influence of Electrospray and Nanoelectrospray on Lithiated Monosaccharide Homodimer Structures Monitored by Differential Ion Mobility Spectrometry-Mass Spectrometry**; Tiffany L Crawford[1]; Gary L. Glish[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC*

METABOLOMICS: GENERAL I
530-549

TP 530 **Development of a Dansyl Labeled Dipeptide Standard Library for Dipeptide Identification Using Dansylation LC-MS Metabolomics Platform**; Kamran Mammadli[1]; Yunong Li[1]; Erik Cardona Gomez[1]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB*

TP 531 **Analysis of Neurotransmitters during Rodent Nervous System Development Using Capillary Electrophoresis-Mass Spectrometry**; Shannon Murphy[1]; Amanda C Weiss[1]; Jennifer W Mitchell[1]; Stanislav S Rubakhin[1]; Martha U Gillette[1]; Jonathan V. Sweedler[1]; *[1]University of Illinois at Urbana Champaign, Urbana, IL*

TP 532 **MIDAS: A Targeted Approach for the Systematic Discovery of Protein-Metabolite Interactions**; Kevin G. Hicks[1]; Aubrie Blevins[1]; Sean R. Hackett[2]; James E. Cox[1,3]; Jared Rutter[1]; *[1]University of Utah School of Medicine, Department of Biochemistry, Salt Lake City, Utah; [2]Calico Life Sciences, South San Francisco, CA; [3]University of Utah Mass Spectrometry & Proteomics Core, Sale Lake City, UT*

TP 533 **High-Throughput Metabolite Profiling of Cell Media for Improved Antibody Production Utilizing a Dual Separation/Mass Spectrometry System with Intelligent MSn Acquisition**; Ioanna Ntai[1]; Anson Pierce[2]; Paul Gulde[2]; Martin Samonig[3]; John Brann[4]; Christopher Elicone[4]; Amanda Souza[1]; Ralf Tautenhahn[1]; Daniel Lopez Ferrer[1]; Andreas Huhmer[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Grand Island, NY; [3]Thermo Fisher Scientific, Germering, Germany; [4]Thermo Fisher Scientific, Franklin, MA*

TP 534 **Metabolomics Uncovers Metabolic Pathways Affected by Glyceryl Trinitrate Treatment: Much More than a Prodrug of Nitric Oxide**; Jan F. Stevens[1]; Elizabeth R. Axton[1]; Jaewoo Choi[2]; *[1]Department of Pharmaceutical Sciences, Linus Pauling Institute, Oregon State University, Corvallis, Oregon; [2]Linus Pauling Institute, Oregon State University, Corvallis, OR*

TP 535 **Unraveling the Effects of Alternaria Toxins on the Rat Metabolome**; Vincent Lüttig[1]; Hannes Puntscher[1]; Mira Flasch[1]; Harald Höger[2]; Doris Marko[1]; Benedikt Warth[1,3,4]; *[1]University of Vienna, Faculty of Chemistry, Department of Food Chemistry and Toxicology, Vienna, Austria; [2]Medical University of Vienna, Core Center of Biomedical Research, Austria, Vienna, Austria; [3]Research Network Chemistry Meets Microbiology, University of Vienna, Vienna, Austria; [4]Vienna Metabolomics Center (VIME), Vienna, Austria*

TP 536 **Age Association Analysis between Tricarboxylic Acid Metabolites and Neurocognitive Impairment in Persons Living with HIV**; Sausan Azzam[1]; Corrilynn Hileman[2]; Daniela Schlatzer[1]; Mark R. Chance[1]; Katherine Tassiopoulos[3]; Robert Kalayjian[2]; *[1]Case Western Reserve University, Cleveland, OH; [2]MetroHealth Med Ctr, Cleveland, OH; [3]Harvard T.H. Chan School of Public Health, Boston, MA*

TP 537 **Development of LC-MS/MS Based Genome-wide Metabolomics for Bacteria**; Vanessa Phelan[1]; Manuel Banzhaf[2]; Alison Waller[3]; *[1]University of Colorado, Denver - Anschutz, Aurora, CO; [2]University of Birmingham, Birmingham, United Kingdom; [3]Brock University, St. Catharines, ON*

TP 538 **Comprehensive Discrimination of Triterpenoids in Three Momordica Species Using Targeted LC-MS/MS Based Metabolomics**; Joydeb Chanda[1]; Akanksha Singh[2]; Sayan Biswas[1]; Pulok K Mukherjee[1]; Dipankar Malakar[2]; Manoj Pillai[2]; *[1]School of Natural Product Studies, Jadavpur University, Kolkata, India; [2]SCIEX, Gurgaon, India*

TP 539 **A New HILIC LC/Q-TOF Metabolomics Method with Biologically Important Isomer Separation and Broad Coverage of Metabolite Classes**; Yuqin Dai[1]; Jordy J. Hsiao[1]; *[1]Agilent Technologies, Santa Clara, CA*

TP 540 **Development of More Reproducible and Sensitive Polar Metabolomics Methods**; Sara Violante[1]; Hardik Shah[1]; Yuqin Dai[2]; Steven M Fischer[2]; Justin R Cross[1]; *[1]Memorial Sloan Kettering Cancer Center, New York, NY; [2]Agilent Technologies, Inc., Santa Clara, CA*

TP 541 **Metabolomics for Environmental Monitoring: Developing Tools for Monitoring the Remediation Activity of Microbial Consortia**; Shawn R. Campagna[1]; Amanda L. May[1]; Yongchao Xie[1]; Mandy Michaelsen[2]; Frank Loeffler[1,3]; *[1]University of Tennessee, Knoxville, TN; [2]US Army Corps of Engineers, Seattle, Washington; [3]Oak Ridge National Laboratory, Oak Ridge, TN*

TP 542 **DNA Adductome and Oxidative Stress-Related Metabolome Changes by the Cooked Meat Carcinogen 2-Amino-1-methyl-6-phenylimidazo[4,5-b]pyridine in Human Prostate Cells**; Jingshu Guo[1]; Medjda Bellamri[1]; Scott Walmsley[1]; Christina Brown[1]; Haoqing Chen[1]; Peter W. Villalta[1]; Robert Turesky[1]; *[1]University of Minnesota, Minneapolis, MN*

TP 543 **A Nontargeted Multi-Omics Workflow for Meconium Analysis Using Ultra High-Pressure Liquid Chromatography Coupled to High Resolution Mass Spectrometry (UHPLC-HRMS)**; Atiye Ahmadireskety[1]; Josef Neu[2]; Richard A Yost[1,3]; John A. Bowden[4]; *[1]University of Florida Department of Chemistry, Gainesville, FL; [2]University of florida, Department of Pediatrics, College of Medicine, Gainesville, Fl, United States, Gainesville, FL; [3]University of Florida Department of Pathology, Immunology, and Laboratory Medicine, Gainesville, FL; [4]University of Florida, College of Veterinary Medicine, Department of Physiological Sciences, Gainesville, Fl, United States, Gainesville, FL*

TP 544 **Hydrolysis of Sulfated Steroids, Toxic Endobiotics and Xenobiotics Using Purified Arylsulfatase for Quantitation of Sulfated and Unconjugated Compounds**; Pongkwan Sitasuwan[1]; L. Andrew Lee[1]; *[1]IMCS, Irmo, SC*

TP 545 **Volatile Metabolites Monitoring of Gut Microbiota Using Secondary Electrospray Based Mass Spectrometry Techniques- a Tale of Two Approaches**; Haorong Li[1]; Mengyang Xu[1]; Jiangjiang (Chris) Zhu[2]; *[1]Miami University, Oxford, OH; [2]The Ohio State University, Columbus, OH*

TP 546 **Revealing the Changes in Pulmonary Arterial Smooth Muscle Cells in Patient by Using Multi-Omics Approach**; Dan Li[1,2,3]; Songjie Chen[4]; Marlene Rabinovitch[1,2,3]; Michael Snyder[4]; *[1]Department of Pediatrics, Stanford University School of Medicine, Stanford, CA; [2]Stanford Cardiovascular Institute, Stanford University, Stanford, CA; [3]Vera Moulton*

Wall Center for Pulmonary Vascular Diseases, Stanford University School of Medicine, Stanford, CA; [4]Department of Genetics, Stanford University School of Medicine, Stanford, CA

TP 547 **Development and Systematic Evaluation of Orthogonal LC-MS Platforms for Metabolomics Workflows**; Jim Blasberg[1]; Kevin Ray[1]; Zhiyun Cao[1]; Ben Cutak[1]; Mark Angeles[1]; *[1]MilliporeSigma, St Louis, MO*

TP 548 **Investigation of Metabolite Modifications during Sample Preparation in Chemical Isotope Labeling LC-MS**; Yunong Li[1]; Kamran Mammadli[1]; Erik Cardona Gomez[1]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB*

TP 549 **Metabolomics Approach to Assess Tissue-Specific Metabolic Alterations in Resuscitated Rats after Prolonged Cardiac Arrest**; Muhammad Shoaib[1]; Jaewoo Choi[2]; Tai Yin[1]; Lance B Becker[1]; Junhwan Kim[1]; *[1]Feinstein Institute for Medical Research, Manhasset, NY; [2]Linus Pauling Institute, Oregon State University, Corvallis, OR*

METABOLOMICS: UNTARGETED METABOLITE PROFILING
550-568

TP 550 **Identification of Type 2 Diabetes Metabolic Biomarkers Based on Chemical Isotope Labeling LC-MS**; Xinyun Gu[1]; Ahmad Aljadaa[2]; Anas Abdel Rahman[2,3,4]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB; [2]College of Medicine, Al Faisal University, Riyadh, Saudi Arabia; [3]King Faisal Specialist Hospital and Research Center, King Faisal Specialist Hospital and Research Center, Saudi Arabia; [4]Memorial University of Newfoundland, St. John's, NL*

TP 551 **Metabolomics Profiling of 5XFAD Mice Model Using Optimized Label-free Untargeted Metabolomics Pipeline**; Boer Xie[1]; Haiyan Tan[2]; Junmin Peng[2]; *[1]St.Jude Children's Research Hospital, Memphis, TN; [2]St Jude Children's Research Hospital, Memphis, TN*

TP 552 **Fast Detection of Pesticides and Drugs Removed from Waste Water by Plants Using Flow Injection Analysis Magnetic Resonance Mass Spectrometry**; Claire Villette[1]; Matthias Witt[2]; Aiko Barsch[2]; Louis Maljers[3]; Dimitri Heintz[4]; *[1]University of Strassbourg, Strassbourg, France; [2]Bruker Daltonik GmbH, Bremen, Germany; [3]Bruker Daltonics Inc., Billerica, MA; [4]University of Strasbourg, Strasbourg, France*

TP 553 **Identification of Antifungal Natural Products in Scab Resistant Pecan Trees**; Zhentian Lei[1]; Clayton D. Kranawetter[1]; Barbara Sumner[1]; Andrew L. Thomas[1]; Santosh Kumar[1]; Lloyd W. Sumner[1]; *[1]University of Missouri, Columbia, MO*

TP 554 **High-resolution Mass Spectrometry for Monitoring Physiological Impacts and Biotransformation Products in Fish Exposed to Wastewater Effluent**; Jonathan Mosley[1]; Marina Evich[2]; Ioanna Ntai[3]; Drew Ekman[1]; Jenna Cavallin[4]; Daniel Villeneuve[4]; Gerald Ankley[4]; Timothy Collette[1]; *[1]US EPA, Athens, GA; [2]ORISE Fellow, US EPA, Athens, GA; [3]Thermo Fisher Scientific, San Jose, California; [4]US EPA, Duluth, MN*

TP 555 **Profiling Weaning Piglet Serum Metabolomic Affected by Acute Exposure of High Concentrations Atmospheric Hydrogen Sulfide**; Zhen Liu[1]; Qingshi Meng[1]; Qixiang Miao[1]; Yanjiao Xie[1]; Hongfu Zhang[1]; Xiangfang Tang[1]; *[1]Institute of Animal Science, Chinese Academy of Agricultural Sciences, Beijing, China*

TP 556 **Metabolomic Profiling of Potential Bioactive Minor Compounds in Amazonian Vegetable Oils and Butters by UHPLC-MSE**; Malra Fasciotti[1]; Michael Murgu[2]; Thays V. C. Monteiro[1]; Simone C. Chiapetta[3]; Alessandra Sussulini[4]; Marcos N. Eberlin[4]; Valnei S. Cunha[1]; *[1]INMETRO, Duque De Caxias, Brazil; [2]Waters Corporation, Barueri, Brazil; [3]National Institute of Technology, Rio de Janeiro, Brazil; [4]University of Campinas, Campinas, Brazil*

TP 557 **Ethanol-Induced Metabolomic Differences in Mice Using HRAM Q-TOF Analysis**; Stephane Moreau[1]; Georgios Theodoridis[2]; Helen G. Gika[3]; Christina Virgiliou[2]; Olga Deda[3]; Ian D Wilson[4]; Neil J Loftus[5]; *[1]Shimadzu Europa GmbH, Duisburg, Germany; [2]Chem and BIOMIC_AUTh, Aristotle University, Thessaloniki, Greece; [3]Medicine and BIOMIC_AUTh, Aristotle University, Thessaloniki, Greece; [4]Imperial College London, Department of Surgery and Cancer, United Kingdom; [5]Shimadzu MS/BU, Manchester, United Kingdom*

TP 558 **Fast Profiling of Tryptophan Metabolites in a Gut Microbiome Study Using Wide Isolation Strategies for UHPLC-HRMS/MS**; Vanessa Y. Rubio[1]; Joy G. Cagmat[1]; Gary P. Wang[1]; Richard A Yost[1]; Timothy J Garrett[1]; *[1]University of Florida, Gainesville, FL*

TP 559 **Metabolomics of *Fusarium verticillioides* / Maize Interaction**; Mark Busman; *USDA, ARS, NCAUR, BFP, Peoria, IL*

TP 560 **Improved Metabolite Identification in a Single Injection with SWATH® Acquisition for Untargeted Metabolomics Workflow**; Robert Proos[1]; Khatereh Motamedchaboki[2]; *[1]Sciex, Framingham, MA; [2]Sciex, Redwood City, CA*

TP 561 **A Collisional Cross Section Database for Diverse Small Molecules: Improving Annotation of Metabolomics Data**; Corey D Broeckling[1]; Jessica E. Prenni[1]; Robert S Plumb[2]; Giorgis Isaac[2]; Johannes PC Vissers[3]; *[1]Colorado State University, Fort Collins, CO; [2]Waters Corporation, Milford, MA; [3]Waters Corporation, Wilmslow, United Kingdom*

TP 562 **Volatile Interactions between *Solanum licopersicum* and *Phytophthora infestans***; Lida Garzón; *Universidad de los Andes, Bogotá D.C, Colombia*

TP 563 **Metabolomics Study of Human Blood Plasma Using 95% 13C Internal Standard with Liquid Chromatography and Ion Mobility-Mass Spectrometry**; Robin H.J. Kemperman[1]; Chris W.W. Beecher[2]; Timothy J. Garrett[1]; Richard A Yost[1]; *[1]University of Florida, Gainesville, FL; [2]IROA Technologies LLC, Bolton, MA*

TP 564 **Multi-omic Discovery of Metabolic Rewiring in Triple-negative Breast Cancer Following Mitochondrial Folate Transport Ablation: Strategy to Reveal Drug-targetable Synthetic Lethalities**; Qiuying Chen[1]; Joshua B Zuk[1]; miller A Christine[2]; Steven M Fischer[2]; Steven Gross[1]; *[1]Weill Medical College of Cornell, New York, NY; [2]Agilent Technologies, Inc., Santa Clara, CA*

TP 565 **Metabolomics Rosetta Stone: Testing Strategies for Harmonization of Untargeted Metabolomics Data Across Multiple Analytical Platforms**; Ken Liu[1]; Vilinh Tran[1]; Chunyu Ma[1]; Karan Uppal[1]; Dean Jones[1]; *[1]Emory School of Medicine, Atlanta, GA*

TP 566 **High-Performance Chemical Isotope Labeling LC-MS for Discovery of Metabolite Biomarkers of Rheumatoid Arthritis**; Xiaohang Wang[1]; Walter P. Maksymowych[1]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB*

TP 567 **Metabolomics Data in the XCMS Cloud: a Resource for Meta Analysis and Systems Biology**; Amelia Palermo[1]; Tao Huan[2]; Duane Rinehart[1]; Markus M Rinschen[1]; Paul H Benton[1]; Eoin Fahy[3]; Shuzhao Li[4]; Shankar Subramaniam[3]; Gary Siuzdak[1,5]; *[1]The Scripps Center for Metabolomics, The Scripps Research Institute, La Jolla, CA; [2]Department of Chemistry, University of British Columbia, Vancouver, BC; [3]Department of Bioengineering, University of California San Diego, La Jolla, CA; [4]Department of Medicine, School of Medicine, Emory University, Atlanta, GE; [5]Department of Chemistry, Molecular and Computational Biology, The Scripps Research Institute, La Jolla, CA*

TP 568 **Metabolomics Characterization of Cell Culture Media by Ultra High Resolution LC-QTOF-MS Analysis**; Xuejun Peng[1]; Guillaume Tremintin[1]; Anjali Alving[2]; Heiko

Neuweger[3]; Aiko Barsch[3]; Nikolas Kessler[3]; [1]*Bruker Daltonics Inc., San Jose, CA;* [2]*Bruker Daltonics Inc., Billerica, MA;* [3]*Bruker Daltonik GmbH, Bremen, Germany*

PHOSPHOPEPTIDES: QUANTITATIVE ANALYSIS
569-579

TP 569 **Global Quantification of Proteome and Phosphoproteome Revealed Novel Cellular Signaling Mechanisms Responsive to Hypoxia and Iron Deficiency**; Luke Erber[1]; Yao Gong[1]; Maolin Tu[1]; Phu Tran[1]; Yue Chen[1]; [1]*University of Minnesota, Minneapolis, MN*

TP 570 **Combining the TMT Calibrator Approach and Immunoaffinity Enrichment for Phosphotyrosine Profiling To Reduce Sample Input Requirements**; Bin Fang[1]; Victoria Izumi[1]; Lily Remsing Rix[1]; Eric Haura[1]; Uwe Rix[1]; Ian Pike[2]; John Koomen[1]; [1]*H. Lee Moffitt Cancer Center, Tampa, FL;* [2]*Proteome Sciences plc, London, United Kingdom*

TP 571 **Analyzing the Neuronal Phosphoproteome: A Systematic Comparison of Fusion Lumos and timsTOF Pro data**; Kristina Desch[1]; Thomas Kosinski[2]; Scarlet Koch[2]; Heiner Koch[2]; Erin M. Schuman[1]; Julian Langer[1,3]; [1]*Max Planck Institute for Brain Research, Frankfurt am Main, Germany;* [2]*Bruker Daltonik GmbH, Bremen, Germany;* [3]*MPI for Biophysics, Frankfurt Am Main, Germany*

TP 572 **Phosphoproteomics with LC-FAIMS Separations Coupled to a Modified Tribrid Orbitrap Mass Spectrometer**; Alexander S. Hebert[1]; Romain Huguet[2]; Graeme C. McAlister[3]; Derek J. Bailey[3]; Michael W. Belford[3]; Michael S Westphall[1]; Joshua J. Coon[1,4,5,6]; [1]*Genome Center of Wisconsin, Madison, WI;* [2]*Thermo Fisher Scientific, San Jose, California;* [3]*Thermo Fisher Scientific, San Jose, CA;* [4]*Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI;* [5]*Department of Chemistry, University of Wisconsin-Madison, Madison, WI;* [6]*Morgridge Institute for Research, Madison, WI*

TP 573 **Quantitative, Comprehensive Multi-Pathway Signaling Analysis Using an Optimized Phosphopeptide Enrichment Method Combined with an Internal Standard Triggered Targeted MS Assay**; Bhavin Patel[1]; Penny Jensen[1]; Aaron S. Gajadhar[2]; Sebastien Gallien[3]; Jae Choi[1]; Romain Huguet[2]; Graeme McAlister[2]; Derek Bailey[2]; Shannon Eliuk[2]; Markus Kellmann[4]; Tabiwang N. Arrey[4]; Alexander Harder[4]; Andreas Huhmer[2]; Kay Opperman[1]; John C Rogers[1]; [1]*Thermo Fisher Scientific, Rockford, IL;* [2]*Thermo Fisher Scientific, San Jose, CA;* [3]*Thermo Fisher Scientific, Precision Medicine Science Center, Cambridge, MA;* [4]*Thermo Fisher Scientific, Bremen, Germany*

TP 574 **Optimization and Implementation of a TMT-based Quantitative Phosphoproteomics Workflow to Identify MELK Substrates**; Joshua Beri[1,2]; Ian M McDonald[2]; Alex Prevatte[1,2]; Dennis Goldfarb[1,3]; Lee M Graves[1,2,3]; Laura E Herring[1,2]; [1]*UNC Proteomics Core Facility, Chapel hill, NC;* [2]*UNC Department of Pharmacology, University of north Carolina at Chapel Hill, Chapel Hill, North Carolina;* [3]*Lineberger Comprehensive Cancer Center, University of North Carolina at Chapel Hill, Chapel Hill, NC*

TP 575 **Evaluation of Spatiotemporal Influences of Interleukin Family- IL-1: Interleukin-33 (IL-33) on Cellular Signal Transduction Pathways**; Rex D a b[1]; Sneha M Pinto[1]; T. S Keshava Prasad[1]; [1]*Yenepoya University, Mangalore, India*

TP 576 **Proteomic and Phosphoproteomic Network Analysis in Alzheimer's Disease**; Lingyan Ping[1,2]; Eric B Dammer[1,2]; Duc M Duong[2,3]; Marla Gearing[2]; James J. Lah[2,4]; Allan I. Levey[2,4]; Nicholas T. Seyfried[1,2,4]; [1]*Department of Biochemistry, Emory University, Atlanta, GA;* [2]*Center for Neurodegenerative Diseases, Emory School of Medicine, Atlanta, GA;* [3]*Department of Biochemistry, Emory University, Atlanta, Georgia;* [4]*Department of Neurology, Emory University, Atlanta, GA*

TP 577 **Tandem Mass Tags (TMT) in Global Quantitative Phosphorylation Analysis**; Ling Li[1]; Dongmei Zhang[1]; Belinda Willard[1]; [1]*Cleveland Clinic, Cleveland, OH*

TP 578 **Phosphoproteomics-Based Molecular Subtyping and Kinase Candidate Nomination for Individual Patients of Diffuse-Type Gastric Cancer**; Mengsha Tong[1]; Chunyu Yu[2]; Jinwen Shi[1]; Yi Wang[1]; Tingting Li[2]; Jun Qin[1]; [1]*State Key Laboratory of Proteomics, Joint Laboratory of Gastrointestinal Oncology, Beijing Proteome Research Center, National Center for Protein Sciences, Beijing, China;* [2]*2. Department of Biomedical Informatics, School of Basic Medical Sciences, Peking University Health Science Center, Beijing, China*

TP 579 **Real-Time, High Density Monitoring of pTyr Signaling Targets in Human Tumors Using Heavy Peptide Triggered Targeted Quantitation**; Aaron S Gajadhar[1]; Lauren E Stopfer[2]; Cameron T Flower[2]; Forest M White[2]; Bhavin Patel[3]; Sebastien Gallien[4]; Romain Huguet[1]; Graeme McAlister[1]; Derek Bailey[1]; Shannon Eliuk[1]; Markus Kellmann[5]; Tabiwang N. Arrey[5]; Alexander Harder[5]; Daniel Lopez Ferrer[1]; Andreas Huhmer[1]; [1]*Thermo Fisher Scientific, San Jose, CA;* [2]*Department of Biological Engineering, Koch Institute for Integrative Cancer Research, Center for Precision Cancer Medicine, Massachusetts Institute of Technology, Cambridge, MA;* [3]*Thermo Fisher Scientific, Rockford, IL;* [4]*Thermo Fisher Scientific, Paris, France;* [5]*Thermo Fisher Scientific, Bremen, Germany*

PROTEIN THERAPEUTICS: QUANTITATIVE ANALYSIS II
580-605

TP 580 **Benchmarking Host Cell Protein Quantification: Label-free vs. a Labeled Global Standard**; Harsha Gunawardena[1]; Jeffrey Brelsford[1]; Melissa Smith[1]; Kevin D. Smith[2]; Hirsh Nanda[2]; [1]*Janssen Research & Development, Spring House, PA;* [2]*Janssen Research and Development, Spring House, PA*

TP 581 **Quantitation of Host Cell Contaminants in Biotherapeutic IgG using LC-ToF-MRM with SILAC Labeled Reference Standards**; Tyler Fletcher[1]; Marla Popov[2]; Stuart Haslam[3]; Ron Orlando[1,2]; [1]*University of Georgia, Athens, GA;* [2]*Glycoscientific LLC, Athens, GA;* [3]*Imperial College, London, United Kingdom*

TP 582 **Immunocapture-LC/MS and LBA-Based Assays as Complementary and Orthogonal Tools for Developing Fusion Protein Therapeutics**; Susan Chen; *Takeda Pharmaceuticals, Inc., Cambridge, MA*

TP 583 **Validation of Amino Acid-Based Isotope Dilution LC-MS/MS Quantification of Insulin Standard Solution Using Sulfur-Based Isotope Dilution ICP/MS**; Hwijin Kim[1,2]; Ji-Seon Jeong[1,2]; Thi Thanh Huong Tran[1,2]; Youngran Lim[2]; Sung Woo Heo[2]; Yong-Hyeon Yim[1,2]; [1]*University of Science and Technology (UST), Daejeon, South Korea;* [2]*KRISS, Daejeon, South Korea*

TP 584 **Impact of Endogenous Biotin on Streptavidin Based Hybrid LBA-LC/MS Assays for Biotherapeutics**; Eric Ma[1]; Moucun Yuan[1]; William R Mylott Jr[1]; [1]*PPD, Richmond, VA*

TP 585 **Biotransformation of Challenging New Modalities – Characterization and Quantitation of Antibody Variant Fragmentation using Affinity Capture Coupled to LC-MS or CE-LIF**; Cong Wu[1]; William Sawyer[1]; Phillip Chu[1]; Neha Srikumar[2]; Nga Tang[1]; Pamela Chan[1]; Gloria Meng[1]; Brian Roper[3]; Thomas Niedringhaus[3]; John Tran[1]; [1]*Biochemical and Cellular Pharmacology, Genentech, Inc., South San Francisco, CA;* [2]*University of Pennsylvania, Philadephia, PA;* [3]*Protein Analytical Chemistry, Genentech, Inc., South San Francisco, CA*

TP 586 **Multi Attribute Monitoring in Therapeutic Glycoprotein Process Development: Benchmark of Different Sample Preparation, Mass Spectrometry Platform and Data**

Processing Software; Bertaccini Diego; *Merck KGaA Darmstadt, Germany, Corsier-sur-Vevey, Switzerland*

TP 587 **SI-traceable quantification of an anti-CD20 monoclonal antibody by Isotope Dilution Mass Spectrometry (IDMS)**; Wei Mi[1]; Zhishang Hu[1]; Yan Chen[2]; *[1]National institute of metrology,China, Beijing, China; [2]Hunan normal university, Changsha, China*

TP 588 **Introducing MA-PAT: a Multi Attribute-Process Analytical Technology to Monitor Protein Quality/ Quantity and Process Characteristics during Biopharma Production**; Jérôme Haustant[1]; Sandrine Fisch[1]; Jérémy Peyrol[1]; Emilie Navarro[1]; Vivien Le Bras[1]; Cédric Mesmin[1]; *[1]Merck Biodevelopment, Martillac, France*

TP 589 **Employing the MS-based Multi-Attribute Method (MAM) for Automated Quality Monitoring of Biotherapeutics**; John N McCarter[1]; Joe Shambaugh[2]; Aude Tartiere[3]; Albert Van Wyk[4]; Cassandra Wigmore[5]; Peter Haberl[6]; *[1]Genedata, Inc., Lexington, MA; [2]Genedata Inc, Lexington, MA, USA, Lexington, Massachusetts; [3]Genedata, San Francisco, CA; [4]Genedata Ltd, Cambridge, UK, Cambridge, United Kingdom; [5]Genedata AG, Basel, Switzerland, Basel, Switzerland; [6]Genedata GmbH, Munich, Germany, Munich, Germany*

TP 590 **Ultra-Sensitive Intact Monoclonal Antibody Quantification Using Automated Sample Preparation Platform and High-Resolution Mass Spectrometer**; Xi Qiu[1]; Wendi Hale[1]; David Wong[2]; *[1]Agilent Technologies, Wilmington, DE; [2]Agilent Technologies, Santa Clara, CA*

TP 591 **A High Resolution Accurate Mass Multi-Attribute Method for Critical Quality Attribute Monitoring and New Peak Detection**; Haichuan Liu[1]; John Rontree[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

TP 592 **Monitoring Multiple Attributes of Biotherapeutics at Peptide Level Using a Single Quadrupole LC/MS for Quality Control**; Linfeng Wu[1]; Lisa Zang[1]; Guannan Li[1]; *[1]Agilent Technologies, Santa Clara, CA*

TP 593 **Comparison between Magnetic Bead and Membrane Immunoaffinity Purification Methods for the Measurement of Monoclonal Antibody in Rat Serum**; Zhiyu Li[1]; Zhiren Yu[1]; Feifei Cui[1]; Weiqun Cao[1]; Lili Xing[1]; Xin Zhang[1]; Yi Tao[1]; *[1]WuXi AppTec, Shanghai, China*

TP 594 **Mass Spectrometric Evaluation of Host Cell Protein Patterns in Biopharmaceutical Products**; Daniel Michael Waldera-Lupa[1]; Thomas Flad[1]; Andreas Dittmar[1]; Heiner Falkenberg[1]; Roland Moussa[1]; *[1]Protagen Protein Services, Dortmund, Germany*

TP 595 **Pre-Clinical Estimation of Cetuximab Using Nano-Surface and Molecular Orientation Limited (nSMOL) Proteolysis and LC-MS/MS**; Deepti Bhandarkar[1]; Rashi Kochhar[1]; Shailendra Rane[1]; Shailesh Damale[1]; Ashutosh Shelar[1]; Purushottam Sutar[1]; Anant Lohar[1]; Bhaumik Trivedi[1]; Navin Devadiga[1]; Ajit Datar[1]; Pratap Rasam[1]; Jitendra Kelkar[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

TP 596 **Quantitation of a PEGylated Human Parathyroid Hormone (1-34) Analog in Rat Plasma Using a Hybrid Immunoaffinity Bottom-Up LC-MS/MS Assay**; Jean-Nicholas Mess[1]; Jean-Francois Dupuis[1]; Kevork Mekhssian[1]; Erik Wagner[2]; Amy Wang[2]; Xin Xu[2]; Karim Berrada[3]; Max Moore[3]; Anahita Keyhani[1]; *[1]Altasciences, Laval , QC; [2]National Center for Advancing Translational Sciences, NIH, Rockville, MD; [3]Frederick National Laboratory for Cancer Research - Leidos Biomedical Research, Frederick, MD*

TP 597 **Investigation of Tissue Distributions of Therapeutic Monoclonal Antibody with Cassette Dosing Strategy and Novel LC/MS Based Method**; Jie Pu[1]; Shihan Huo[1]; Chao Xue[1]; Ming Zhang[1,2]; Jun Qu[1,2]; *[1]SUNY, at Buffalo, Buffalo, NY; [2]New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, New York*

TP 598 **Quantitation of CHO Media Nutrients and Metabolites in under 180 seconds by an Integrated CE-MS Analyzer**; Kenion H. Blakeman[1]; Ji Young Anderson[1]; Colin M. Gavin[1]; Drew Blouch[1]; Christopher D. Brown[1]; Glenn A. Harris[1]; *[1]908 Devices, Inc., Boston, MA*

TP 599 **Application of Top Down Degradomics to Guide Development of Stable Antibody Variants**; Phillip Chu[1]; christopher Davies[2]; Cong Wu[2]; Tangsheng Yi[2]; James Koerber[2]; John C. Tran[2]; *[1]Genentech Inc., South San Francisco, CA; [2]Genentech, South San Francisco, CA*

TP 600 **Rapid, Sensitive, and Routine Intact mAb Quantification using a Compact Tof HRMS Platform**; Yun Alelyunas[1]; Henry Shion[1]; Mark D Wrona[1]; Weibin Chen[1]; *[1]Waters Corporation, Milford, MA*

TP 601 **Comprehensive Characterization of Antibody Drug Conjugates Enabled by Top-down and Middle-down Mass Spectrometry Strategies**; Eli J Larson[1]; Bifan Chen[1]; Ziqing Lin[2,3]; Yanlong Zhu[2,3]; Yutong Jin[1]; Qingge Xu[2,3]; Cexiong Fu[4]; Zhaorui Zhang[4]; Qunying Zhang[4]; Wayne A Pritts[4]; Ying Ge[1,2,3]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706; [2]Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; [3]Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI; [4]Process Analytical Chemistry, AbbVie Inc., North Chicago, IL*

TP 602 **Evaluating Stability of Human Monoclonal Antibody in Rat Cell Cultures Using a Surrogate Peptide LC-MS/MS Approach**; Nadya Galeva[1]; Reed Murbach[1]; Krystal Gilligan[1]; Kevin Westland[1]; Seema Muranjan[1]; *[1]Sekisui XenoTech, LLC, Kansas City, KS*

TP 603 **An Integrated LC-MS Platform for Monitoring Quality Attributes of Biotherapeutic Products**; Chengfeng Ren[1]; Frank Macchi[2]; Monica Sadek[2]; Benjamin Moore[2]; *[1]Genentech, South San Francisco, CA; [2]Genentech Inc., South San Francisco, CA*

TP 604 **Non-Labelling Approach for Absolute Quantitation of Total Biotherapeutics and Simultaneous Detection of Blood Volume in Tissues Using LC/MS**; Miho Ayabe[1]; Naoaki Murao[2]; Masaki Ishigai[3]; Hiroyuki Tsunoda[1]; *[1]Chugai Pharmaceutical Co., Ltd., Kamakura, Japan; [2]Chugai Pharmaceutical Co., Ltd., Gotemba, Japan; [3]Chugai Pharmaceutical Co., Ltd., Chuo-ku, Japan*

TP 605 **Limited Tryptic Digestion-Isotope Dilution Mass Spectrometry (LTD-IDMS): An Alternative Potency Assay to Single Radial Immunodiffusion (SRID) for Influenza Vaccines**; Tracie Williams[1]; Hans C Cooper[1]; John R Barr[1]; *[1]Centers for Disease Control and Prevention, Atlanta, GA*

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TP 606 **Taking Charge Variant Analysis to the Next Level: Targeted and Automated Charge Variant-Coupled Native Mass Spectrometry (CV-MS)**; Mauro Sassi[1]; Mara Rossi[1]; Angelo Palmese[1]; *[1]Merck KGaA, Guidonia Montecelio, Italy*

TP 607 **NanoFlow LCMS and Dedicated Bioinformatics Software for Rapid Semi-Automated Biotherapeutics PTM Quantitation**; Tun Liu[1]; Jennifer Nemeth-Seay[2]; Michael Merriman[3]; Sean McCarthy[3]; *[1]Janssen Research & Development, Spring House, PA; [2]Janssen Research and Development, Spring House, PA; [3]Sciex, Framingham, MA*

TP 608 **Characterization of Protein Therapeutics Using ZipChip Microfluidic Capillary Electrophoresis-Mass Spectrometry**; Ekaterina G. Deyanova[1]; Richard Huang[1]; Pradyot Nandi[1]; Priyanka Madia[1]; Guodong Chen[1]; *[1]Bristol-Myers Squibb Company, Princeton, NJ*

TP 609 **Using Hydrogen Exchange-Mass Spectrometry (HX-MS) to Identify Agitation-Induced Unfolding Events Causing Aggregation in Monoclonal Antibodies (mAbs)**; Chamalee D Gamage[1]; David D. Weis[1]; Benjamin Walters[2]; *[1]University of Kansas, Lawrence, KS; [2]Genentech, Inc., South San Francisco, CA*

TP 610 **Analysis of Aggregation-Prone Full-Length Antibodies Using FPOP-LC-MS/MS**; Owen Cornwell[1]; Nicholas J Bond[2]; Sheena E Radford[1]; Alison E Ashcroft[1]; *[1]University of Leeds, Leeds, United Kingdom; [2]MedImmune, Cambridge, United Kingdom*

TP 611 **Assessing the Protein A Binding Affinity of Monoclonal Antibody Variants Using Protein A Chromatography Coupled to Native Mass Spectrometry**; Victoria C. Cotham[1]; Shunhai Wang[1]; Thomas J. Daly[1]; Ning Li[1]; *[1]Regeneron Pharmaceuticals Inc., Tarrytown, NY*

TP 612 **An Efficient LC/MS Workflow for Identification and Monitoring of Host Cell Proteins for Assisting Monoclonal Antibody Purification**; Catalin Doneanu[1]; Malcolm Anderson[2]; Alex Xenopoulos[3]; Romas Skudas[4]; Ying Qing Yu[1]; Asish Chakraborty[1]; Weibin Chen[1]; *[1]Waters Corporation, Milford, MA; [2]Waters Corporation, Wilmslow, United Kingdom; [3]EMD Millipore Corporation, Bedford, MA; [4]Merck KGaA, Darmstadt, Germany*

TP 613 **A Specific and Sensitive LC-MS/MS PRM Method to Quantify C-Terminal Lysine Clipping in Monoclonal Antibodies**; Lei Wang[1]; Mei M Zhu[1]; Charles Nwosu[1]; Anne Kowal[1]; *[1]Takeda Pharmaceuticals, Inc., Cambridge, MA*

TP 614 **A Comprehensive Physicochemical Characterization of an Original and Biosimilar Tenecteplase by Mass Spectrometry Methods**; Maksim Degterev[1]; Maxim Smolov[1]; Alexander Vishnevskiy[1]; Rakhim Shukurov[1]; *[1]IBC Generium, Vol'ginskiy, Russian Federation*

TP 615 **Primary Structures of Intact DTPA-Coupled Recombinant Epidermal Growth Factors can be Evaluated via MS-Based Chemical Formula Verification**; Yen-chun Huang[1]; Yu-Hsuan Lin[1]; Ya-Fen Chen[2]; C Allen Chang[3]; Yeou-Guang Tsay[1,4]; *[1]Institute of biochemistry and molecular biology, National Yang-Ming University, Taipei, Taiwan; [2]Sunjet Co., Ltd., Taipei, Taiwan; [3]Department of Biomedical Imaging and Radiological Sciences, National Yang-Ming University, Taipei, Taiwan; [4]Proteomics Research Center, National Yang-Ming University, Taipei, Taiwan*

TP 616 **Identifying Early Production Truncated Drug Candidates by Top-Down Mass Spectrometry**; Zhe Zhang; *Novartis, Cambridge, MA*

TP 617 **Rapid Critical Quality Attribute Assessment of Biotherapeutic Proteins Using an Automated Top-Down Sequencing LC-MS Workflow**; Matthew Maust[1]; Li Cui[1]; Greg Kilby[1]; Juan Aon[1]; Keegan Orzechowski[1]; Wilfred Tang[2]; Michelle English[2]; Marshall Bern[2]; *[1]GlaxoSmithKline, Collegeville, PA; [2]Protein Metrics Inc., Cupertino, CA*

TP 618 **Characterization of Peptide with Disulfide Bond Linkage on LC Time Scale with Differential Mobility and ECD Fragmentation**; Suya Liu[1]; Yves Le blanc[2]; Doug Simmons[1]; Pavel Ryumin[1]; Takashi Baba[1]; *[1]SCIEX, Concord, ON; [2]SCIEX, Concord, On, ON*

TP 619 **Advancements in Native Analysis by Microchip Capillary Electrophoresis-ESI-MS**; J. Scott Mellors[1]; Ashley Bell[2]; Erin A. Redman[1]; *[1]908 Devices, Inc., Carrboro, NC; [2]908 Devices, Boston, MA*

TP 620 **Novel Analytical Paradigm for Accurate Characterization and Routine Monitoring of Deamidation and Succinimide Intermediate in Biotherapeutic Proteins**; Sergei Saveliev[1]; Mingyan Cao[2]; Sri Hari Raju Mulagapati[2]; Bhargavi Vemulapati[2]; Jihong Wang[2]; Alan Hunter[2]; Marjeta Urh[1]; Dengfeng Liu[2]; *[1]Promega Corporation, Madison, WI; [2]MedImmune, Gaithersburg, MD*

TP 621 **Structural Characterization of Peptide-Loaded Major Histocompatibility Complexes (pMHC) through Top Down Native Mass Spectrometry**; Dhanashri Bagal[1]; Songyu Wang[1]; Bradford W. Gibson[2]; *[1]Amgen, South San Francisco, CA; [2]Amgen, South San Francisco, CA*

TP 622 **Analysis of Antibody Subunits by ETD Parallel Ion Parking on a Chromatographic Timescale**; Joshua D. Hinkle[1]; Emily Zahn[1]; Robert D'Ippolito[1]; Elizabeth Duselis[1]; Dina L. Bai[1]; Jeffrey Shabanowitz[1]; Donald F. Hunt[1]; *[1]University of Virginia, Charlottesville, VA*

TP 623 **High Resolution Separations for Detailed LC/MS Analysis of mAb Disulfide Variants**; Barry Boyes[1]; William E Miles[2]; Ben Libert[1]; *[1]Advanced Materials Technology Inc,, Wilmington, DE; [2]Advanced Materials Technology, Wilmington, DE*

TP 624 **Ultra-Comprehensive Antibody Fc-Fusion Protein Characterization Using a Tribrid Orbitrap Mass Spectrometer Modified for PTR and Extended Mass Range Applications**; Aaron O Bailey[1]; Yi Zeng[1]; Joshua Silveira[2]; Kristina Srzentić[2]; Christopher Mullen[2]; John E. P. Syka[2]; Romain Huguet[2]; Siqi Liu[3]; Guanghui Han[1]; *[1]BGI Americas, San Jose, CA; [2]Thermo Fisher Scientific, San Jose, CA; [3]BGI-Shenzhen, Shenzhen, China*

TP 625 **Not All IgG1 Monoclonal Antibody Disulfide Bonds Are Created Equal**; Andrew Dykstra[1]; Neeraj Agrawal[1]; *[1]Amgen, Thousand Oaks, CA*

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TP 626 **Protein Phosphorylation Landscape of Mouse Spermatids During Spermiogenesis**; Yan Li[1]; Yiwei Cheng[1]; Tianyu Zhu[1]; Hao Zhang[1]; Hui Zhu[1]; Xuejiang Guo[1]; *[1]Nanjing Medical University, Nanjing, China*

TP 627 **Identification and Validation of Calcineurin Interactors**; Brooke Brauer[1]; Sarah Sheftic[2]; Isha Nasa[1]; Thomas Moon[2]; Rebecca Page[2]; Wolfgang Peti[2]; Arminja N Kettenbach[1]; *[1]Dartmouth College, Hanover, NH; [2]University of Arizona, Tucson, AZ*

TP 628 **A Quantitative Chemical Proteomic Analysis of Cysteine Reactivity**; Evan W. McConnell[1]; Leslie M. Hicks[1]; *[1]UNC, Chapel Hill, NC*

TP 629 **Proximity-Dependent Identification of *in vivo* Putative Substrates of Protein Kinases**; Tomoya Niinae[1]; Koshi Imami[1]; Chia-Feng Tsai[2]; Naoyuki Sugiyama[1]; Yasushi Ishihama[1]; *[1]Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, Japan; [2]PNNL, Richland, WA*

TP 630 **High Sensitivity PTM Characterization in Cell Lysates Using Trapped Ion Mobility**; Matthew Willetts[1]; Shourjo Ghose[1]; Gary Kruppa[1]; Matthew P Stokes[2]; Charles Farnsworth[2]; Kimberly Lee[2]; *[1]Bruker Scientific, Billerica, MA; [2]Cell Signaling Technology, Danvers, MA*

TP 631 **Phosphoproteomic Analyses of Multiple Species of Snakes Provides Insight into the Regulation of Intestinal Function and Regeneration**; Abu Hena M Kamal[1]; Blair Perry[1]; Todd Castoe[1]; Stephen M. Secor[2]; Saiful M. Chowdhury[1]; *[1]University of Texas at Arlington, Arlington, TX; [2]University of Alabama, Tuscaloosa, AL*

TP 632 **Proteomics of Diatoms: Discovery of Polyamine Modifications in Biosilica-Associated Proteins**; Alexander Milentyev[1]; Christoph Heintze[2]; Nicole Poulsen[2]; Nils Kroeger[2]; Matthias Wilm[3]; Andrej Shevchenko[4]; *[1]Max Planck Institute of Molecular Cell Biology and Genetics (MPI-CBG), Dresden, Germany; [2]Center for Molecular and Cellular Bioengineering (CMCB), Dresden, Germany; [3]Conway Institute of Biomolecular and Biomedical Research, Dublin, Ireland; [4]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany*

TP 633 **Creating a Functional Map of the Human Phospho-Proteome Using a "Big Data" Approach**; David Ochoa[1]; Andrew F. Jarnuczak[1]; Pedro Beltrao[1]; Juan Antonio Vizcaino[1]; *[1]EMBL-EBI, Hinxton, United Kingdom*

TP 634 **Determining the Phosphorylation Dynamics in Human Spliceosome**; Kuan-Ting Pan[1]; Ivan Silbern[1]; Majety Naga Leelaram[1]; Olexandr Dybkov[1]; Reinhard Luehrmann[1]; Henning Urlaub[1,2]; *[1]Max-Planck Inst for Biophysical Chemistry, Goettingen, Germany; [2]University Medical Center Goettingen (UMG), Goettingen, Germany*

TP 635 **Comprehensive Characterization of Biotherapeutic Degradation *in vivo* Using a Modified Orbitrap Tribrid with Extended Mass Range**; Kristina Srzentic[1]; Romain Huguet[2]; Luca Fornelli[3]; *[1]Thermo Fisher Scientific, Cambridge, MA; [2]Thermo Fisher Scientific, San Jose, CA; [3]University of Oklahoma, Norman, OK*

TP 636 **Combined GluC-Based Middle-Down and Top-Down Proteomics of Histone H4 in a Single Analysis**; Matthew Holt[1]; Tao Wang[1]; Nicolas L Young[1]; *[1]Baylor College of Medicine, Houston, TX*

TP 637 **An Integrated Intact Mass and Bottom-Up Approach to Characterization of New Biologics**; Hirsh Nanda[1]; Bo Zhai[1]; Andrew D Mahan[1]; Harsha P. Gunawardena[1]; Andrew C Nichols[2]; Jing Li[2]; Yong J. Kil[2]; Marshall Bern[2]; Eric Carlson[2]; *[1]Janssen Research & Development, Cell & Developability Sciences, Spring House, PA; [2]Protein Metrics Inc., San Carlos, CA*

TP 638 **Characterization of S-Nitrosylation in Aged Rabbit Using Oxidized Cysteine-Selective cPILOT**; Katarena Ford; *Vanderbilt University, Nashville, TN*

TP 639 **Bothrops Snake Venoms: Glycoproteomic Analysis and the Role of Sialic Acid in Toxin Function.**; Carolina Brás Costa[1,2]; Débora Andrade Silva[1,2]; Daniela Cajado Carvalho[1]; Solange Maria de Toledo Serrano[1]; *[1]Butantan Institute, São Paulo, Brazil; [2]Chemistry Institute -USP, São Paulo, Brazil*

TP 640 **Minimizing Deamidation During the Trypsin Digestion of Proteins**; Paul R Collop[1]; Ron Orlando[2]; *[1]University of Georgia, Athens; [2]University of Georgia, Athens, GA*

TP 641 **A Rapid and Robust Protocol for Disulfide Bond Identification and Validation Using Pepsin/Trypsin Digestion and Spectrum Identification Machine**; Chuanlong Cui[1]; Tong Liu[1]; Annie Beuve[1]; Hong Li[1]; *[1]Rutgers New Jersey Medical School, Newark, NJ*

TP 642 **Analysis of Histones from HEK293 Cells Using a QTOF with Trapped Ion Mobility and PASEF Workflows**; Shourjo Ghose[1]; Matthew Willetts[1]; Miranda Gardner[2]; Michael Freitas[2]; Gary Kruppa[1]; *[1]Bruker Scientific, Billerica, MA; [2]The Ohio State University, Columbus, OH*

TP 643 **Quantitative Proteomics Reveals Differential Huntingtin Ubiquitination and Global Proteome Changes in a Mice Model for Huntington's Disease**; Karen A Sap[1]; Arzu Tugce Guler[1]; Aleksandra Bury[1]; Karel Bezstarosti[2]; Jeroen A.A. Demmers[2]; Eric A. Reits[1]; *[1]Amsterdam UMC, Amsterdam, Netherlands; [2]Erasmus MC, Rotterdam, Netherlands*

TP 644 **The Invisible Link – Connecting Autophagy and Alzheimer's Disease**; Tyler R Lambeth[1]; Dylan L. Riggs[2]; Ryan R. Julian[2]; *[1]University of California-Riverside, Riverside, CA; [2]University of California, Riverside, Riverside, CA*

TP 645 **Orthogonal Approaches for Released N-Glycan Characterization and Quantification**; Sean McCarthy[1]; Zoe Zhang[2]; Elliott Jones[2]; *[1]SCIEX, Framingham, MA; [2]Sciex, Redwood City, CA*

TP 646 **oxSWATH: An Integrative Method for a Comprehensive Redox-Centered Analysis Combined with a Generic Differential Proteomics Screening**; Bruno Manadas[1]; Matilde Melo[1]; Liliana R Loureiro[1]; Mário Grãos[1]; Pedro Castanheira[2]; Sandra I. Anjo[1]; *[1]Center for Neuroscience and Cell Biology, Cantanhede, Portugal; [2]Biocant, Cantanede, Portugal*

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TP 647 **Bacterial Identification Using Machine Learning Defined Peptide Signatures and its Validation by a Targeted Proteomics Approach under Routine Conditions**; Clarisse Gotti-Barban[1]; Florence Roux-Dalvai[1]; Mickael Leclercq[1]; Frédéric Fournier[1]; Marie-Claude Hélie[2]; Judith Marcoux[1]; Isabelle Kelly[1]; Tabiwang N. Arrey[3]; Cristina C. Jacob[4]; Claire Dauly[3]; Claudia P.B. Martins[4]; Julie Bestman-Smith[5]; Maurice Boissinot[2]; Michel G. Bergeron[2]; Arnaud Droit[1]; *[1]Proteomics Platform, CHU de Québec Research Centre, Laval University, Québec, QC; [2]Infectiology Research Centre, CHU de Québec, Laval University, Québec, QC; [3]Thermo Fisher Scientific, Bremen, Germany; [4]Thermo Fisher Scientific, San Jose, CA; [5]Enfant-Jésus Hospital, CHU de Québec, Laval University, Québec, QC*

TP 648 **Dynamic Bovine Milk Proteome Alterations during *Staphylococcus aureus* Infection in Subclinical and Clinical Mastitis**; Kiran Ambatipudi[1]; Sudipa Maity[1]; Debiprasanna Das[2]; *[1]Indian Institute of Technology Roorkee, Roorkee, India; [2]College of Veterinary Science and Animal Husbandry, Bhubaneswar, India*

TP 649 **Identifying the Molecular Mechanisms of Sex-Specific Severity of the Middle East Respiratory Syndrome Coronavirus (MERS-CoV) Using Proteomics**; Natarajan Bhanu[1]; Simone Sidoli[1]; Ranran Wu[1]; Neeltje van Doremalen[2]; Vincent Munster[2]; Angela Rasmussen[3]; Benjamin A. Garcia[4]; *[1]University of Pennsylvania, Philadelphia, PA; [2]National Institutes of Health, Rocky Mountain Laboratories, Hamilton, MT; [3]Columbia University Mailman School of Public Health, New York City, NY; [4]University of Pennsylvania, Philadephia, PA*

TP 650 **Quantitative Proteomics Analyses of Neuronal Cells Exposed to HIV-1 Infected MDM Supernatants with High Cathepsin B Secretion**; Camille N. Zenon[1]; Estheisy Roman[2]; Abiel Roche Lima[1]; Kelvin Carrasquillo Carrión[1]; Yadira M Cantres Rosario[1]; Loyda M. Melendez[1]; *[1]University of Puerto Rico Medical Sciences Campus, San Juan, PR; [2]Universidad del Este, Carolina, Puerto Rico*

TP 651 **Dynamic Proteomic Profiling of the Salmonella-Host Interplay Reveals New Modes of Action for Known and Novel Virulence Factors**; Jennifer Geddes-McAlister[1]; Stefanie Vogt[2]; Jennifer Rowland[2]; Sarah Woodward[2]; Baerbel Raupach[3]; Brett Finlay[2]; Felix Meissner[1]; *[1]University of Guelph, GUELPH, ON; [2]University of British Columbia, Vancouver, BC; [3]Max Planck Institute for Infectious Biology, Berlin, Germany; [4]Max Planck Institute of Biochemistry, Martinsried, Germany*

TP 652 **New Insights in Formaldehyde-Induced Detoxification of the Tetanus Toxin: Chemical Modification Stoichiometry and Characterization of Intra- and Inter-Molecular Cross-Links**; Nour AL Turihi[1,2]; Sébastien Peronin[2]; Arnaud Salvador[1]; Fabien Barbirato[3]; Vincent Colombie[3]; Céline Rocca[3]; Catherine Jourdat[3]; Thierry Eynard[2]; Jérôme Lemoine[1]; *[1]Institut des Sciences Analytiques, UMR 5280 CNRS Université Lyon 1, Université de Lyon, Villeurbanne, France; [2]MTech, Sanofi Pasteur, Neuville-sur-Saône, France; [3]Sanofi Pasteur, Marcy l'Etoile, France*

TP 653 **Analysis of *Staphylococcus aureus* Infections through Spatially Targeted Micro-Proteomics**; Daniel Ryan[1,2]; Nathan H. Patterson[2,3]; James E. Cassat[4,5,6,7]; Eric P. Skaar[1,7,8]; Richard M. Caprioli[1,2,3,9,10]; Jeffrey M. Spraggins[1,2,3]; *[1]Department of Chemistry, Vanderbilt University, Nashville, TN; [2]Mass Spectrometry Research*

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TP 654 **Challenges in Clinical Metaproteomics Highlighted by the Analysis of Acute Leukemia Patients with Gut Colonization by Multidrug-Resistant *Entero bacteriaceae***; Julia Rechenberger[1]; Patroklos Samaras[1]; Anna Jarzab[1]; Juergen Behr[2]; Martin Frejno[1]; Ana Djukovic[5]; Jaime Sanz[4, 5]; Eva M. González-Barberá[4]; Miguel Salavert[4]; Jose Luis López-Hontangas[4]; Karina B. Xavier[6]; Laurent Debrauwer[7, 8]; Jean-Marc Rolain[9]; Miguel Sanz[4, 5]; Marc Garcia-Garcera[10]; Mathias Wilhelm[1]; Carles Ubeda[3, 11]; Bernhard Kuster[1, 2]; *[1]Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; [2]Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany; [3]Centro Superior de Investigación en Salud Pública-FISABIO, Valencia, Spain; [4]Hospital Universitari i Politècnic La Fe, Valencia, Spain; [5]CIBERONC, Instituto Carlos III, Madrid, Spain; [6]Instituto Gulbenkian de Ciência, Oeiras, Portugal; [7]Toxalim, Université de Toulouse, INRA, INP-ENVT, INP-EI-Purpan, Université de Toulouse 3 Paul Sabatier, Toulouse, France; [8]Axiom Platform, UMR 1331 Toxalim, MetaToul-MetaboHUB, National Infrastructure of Metabolomics and Fluxomics, Toulouse, France; [9]Aix Marseille Univ, IRD, APHM, MEPHI, IHU-Méditerranée Infection, Marseille, France; [10]Department of Fundamental Microbiology, University of Lausanne, Lausanne, Switzerland; [11]Centers of Biomedical Research Network (CIBER) in Epidemiology and Public Health, Madrid, Spain*

TP 655 **Analysis of Zika Viral Polyprotein N- and O-glycosylation Using a Novel Lectin-chemoenzymatic Enrichment**; Shuang Yang[1]; Felipe Assis[1]; Wells W. Wu[1]; Johnathan Sjögren[2]; Lisa Parsons[1]; Helén Nyhlén[2]; Philip Onigman[3]; Rong-Fong Shen[1]; Maria Rios[1]; John F. Cipollo[1]; *[1]CBER, FDA, Silver Springs, MD; [2]Genovis AB, Lund, Sweden; [3]Genovis Inc., Cambridge, MA*

TP 656 **Comprehensive Analysis of the Human Cytomegalovirus Interactome to Identify Key Hubs of Protein Degradation**; Luis Nobre[1]; Katie Nightingale[1]; Benjamin J Ravenhill[1]; Robin Antrobus[1]; Gavin W.G. Wilkinson[2]; Richard J Stanton[2]; Edward L Huttlin[3]; Michael Weekes[1]; *[1]University of Cambridge, Cambridge, United Kingdom; [2]University of Cardiff, Cardiff, United Kingdom; [3]Harvard Medical School, Boston, MA*

TP 657 **Scalable Proteomic Analysis of Microbes (SPAM): A New Weapon in the Global Fight Against Antimicrobial Resistance**; Annegret Ulke-Lemee[1]; Thomas Rydzak[1]; Laurent Brechenmacher[1]; Soren Wacker[1]; Troy Feener[1]; Mario E. Valdes-Tresanco[1]; Tara Winstone[2]; Sergei Y. Noskov[1]; Deirdre Church[2]; Ian A. Lewis[1]; *[1]University of Calgary, Calgary, AB; [2]Calgary Laboratory Services, Calgary, AB*

PROTEOMICS: INTACT PROTEINS
658-666

TP 658 **Multiple Ion Chromatogram (MIC) for Direct Quantification of Intact Proteins Using Q-TOF Mass Spectrometry**; Yonghai Lu[1]; Jie Xing[1]; Djohan Kesuma[1]; Zhaoqi Zhan[1]; *[1]Shimadzu Asia Pacific, Singapore, Singapore*

TP 659 **Impaired Degradation Dynamics of Synaptic Vesicle Machinery in APPKI Mice**; Nalini R Rao[1]; Ewa Bomba-warczak[1]; Timothy Hark[1]; Jeffrey N. Savas[1]; *[1]Northwestern University, Chicago, IL*

TP 660 **Mass Spectrometry in the Development of Better Coagulation Tests: Quantitation and Proteoform Characterization of Antithrombin**; Renee Ruhaak[1]; Fred P.H.T.M. Romijn[1]; Mervin Pieterse[1]; Jan Nouta[1]; Nico Smit[1]; Elena Dominguez-Vega[1]; Yuri E.M. van der Burgt[1]; Manfred Wuhrer[1]; Christa M. Cobbaert[1]; *[1]LUMC, Leiden, Netherlands*

TP 661 **The Strange Case of "Picket Fence" Peaks: A Study in the Complexity of MS/MS Spectra of Protein Ions**; John E. P. Syka[1]; Joshua D. Hinkle[2]; Christopher Mullen[1]; Robert D'Ippolito[2]; Romain Huguet[1]; Lissa C. Anderson[3]; Jeffrey Shabanowitz[2]; Donald F. Hunt[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]University of Virginia, Charlottesville, VA; [3]NHMFL, Florida State Univ., Tallahassee, FL*

TP 662 **A Direct Computational Approach to the Analysis of Multiply Charged Biomolecules and Their Modifications with Electrospray Mass Spectrometry**; Ning Zhang[1]; Shundi Shi[2]; Shenglong Zhang[1]; David Good[3]; Don Kuehl[4]; Yongdong Wang[4]; *[1]Department of Life Sciences, New York Institute of Technology, New York, NY; [2]Department of Chemical Engineering, Columbia University, New York, NY; [3]Covance Laboratories Inc., Madison, WI; [4]Cerno Bioscience, Norwalk, CT*

TP 663 **Top-down Proteomics and Metabolomics based Profiling and Characterization of Collagen by LC-QTOF-MS**; Tao Jiang[1]; Todd Osiek[1]; Xuejun Peng[2]; *[1]Mallinckrodt, Hazelwood, MO; [2]Bruker Daltonics Inc., San Jose, CA*

TP 664 **Liquid Chromatography – Triple Quadrupole Mass Spectrometry for Top-Down Quantitative Analysis of Low Abundance Intact Proteins from Biological Samples**; Katarina Marakova[1]; Joshua Lee Isaacs[2]; Alex J Rai[3]; Kevin A Schug[2]; *[1]Comenius University in Bratislava, Bratislava, Slovakia; [2]The University of Texas at Arlington, Arlington, TX; [3]Columbia University, New York, NY*

TP 665 **1400 Proteoforms Identified from Five Micrograms of Escherichia coli Proteins Using Online 2D pH RP/RPLC Top-Down Mass Spectrometry**; Zhe Wang[1]; Dahang Yu[1]; Xiaowen Liu[2]; Kenneth Smith[3]; Si Wu[1]; *[1]University of Oklahoma, Norman, OK; [2]IUPUI, Indianapolis, IN; [3]Oklahoma Medical Research Foundation, Oklahoma City, OK*

TP 666 **"Intact Preteomictrum" from Intact-Protein List between 10kDa to 200kDa in Eukaryotic Cell with in Trap-MALDI Mass Spectrometer**; Shih-Chieh Yang[1]; Szu-Wei Chou[1]; Yi-Teng Hsiao[1]; pin-duo lee[1]; *[1]AcroMass technologies, Inc., Taipei, Taiwan*

PROTEOMICS: NEW APPROACHES I
667-694

TP 667 **Toward Robust and High-Throughput Single Cell Proteomics Based on TMT Based Nanodroplet Sample Processing and Ultrasensitive LC-MS**; Maowei Dou[1]; Geremy C. Clair[1]; William B. Chrisler[1]; Kerui Xu[1]; Ryan L. Sontag[1]; Rui Zhao[1]; Ronald J. Moore[1]; Derek Bailey[2]; Greg A. Foster[2]; Daniel Lopez-Ferrer[2]; Richard D. Smith[1]; Wei-Jun Qian[1]; Ryan T. Kelly[1, 3]; Charles K. Ansong[1]; Ying Zhu[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Thermo Fisher Scientific, San Jose, CA; [3]Brigham Young University, Provo, UT*

TP 668 **Application of Probabilistic Information Retrieval for Ultra Rapid Peptide Sequencing Utilizing Comprehensive Protein Isoform Databases**; Jeffrey J. Jones[1]; Ryan Benz[1]; *[1]SoCal Bioinformatics Inc., Montrose, CA*

TP 669 **Extremely Long-Lived Mitochondrial Proteins in Neuronal Health and Aging**; Ewa Bomba-warczak[1]; Jeffrey N. Savas[1]; *[1]Northwestern University, Chicago, IL*

TP 670 **Single Cell Proteomic Analysis Using PASEF**; Catherine C L Wong; *Center for Precision Medicine Multiomics Research, Peking University, Beijing, China*

TP 671 **Enriching Low Abundance APEX2 Biotin Modifications from Complex Mixtures**; Morgan Hepburn[1]; Frances Snider[1]; James D McGhee[1]; David C Schriemer[1]; *[1]University of Calgary, Calgary, AB*

TP 672 **Spatiotemporally-Precise Proximity Proteomics Reveals Nuclear Lamina-Peripheral Chromatin Interactome *in vivo***; Xi Zhang[1]; Kanishk Abhinav[2]; Tess Branon[3]; Alice Ting[3]; John R. Yates, III[2]; Larry Gerace[2]; *[1]Scripps, La Jolla; [2]Scripps Research, La Jolla, CA; [3]Stanford University, Stanford, CA*

TP 673 **Ultra-Fast Proteomics Enabled by Scanning SWATH and High-Flow Chromatography**; Christoph B Messner[1]; Vadim Demichev[2,3]; Spyros Vernardis[3]; Nic Bloomfield[4]; Gordana Ivosev[4]; Fras Wasim[4]; Stephen Tate[4]; Kathryn Lilley[2]; Markus Ralser[3,5]; *[1]Francis Crick Institute, London, United Kingdom; [2]Department of Biochemistry, University of Cambridge, Cambridge, United Kingdom; [3]The Francis Crick Institute, London, United Kingdom; [4]SCIEX, Concord, ON; [5]Charité, Berlin, Germany*

TP 674 **Proteomic Analysis of *Rhizopus microsporus* IOC4686 Fungus Isolated from Mining Environment: Screening for Protein Biomarkers Induced by Copper**; Meriellen Dias[1]; Thalles Jocelino Gomes de Lacerda[2]; Lidiane Maria Andrade[1]; Claudio Augusto Oller do Nascimento[1]; Enrique Eduardo Rozas Sanchez[1]; Maria Anita Mendes[1]; *[1]Dempster MS Lab- Poli-USP, Sao Paulo, Brazil; [2]Federal University of São Paulo, Sao Paulo-SP, Brazil*

TP 675 ***Chlorella vulgaris* Microalgae: Proteomic Changes Due to Copper**; Lidiane Maria de Andrade[1]; Meriellen Dias[2]; Cristiano José de Andrade[3]; Maria Anita Mendes[2]; Jorge Alberto Soares Tenório[4]; Claudio Augusto Oller Nascimento[2]; *[1]Dempster MS Lab- Poli-USP, São Paulo, Brazil; [2]Dempster MS Lab- Poli-USP, Sao Paulo, Brazil; [3]LiEB – Integrated Laboratory of Biological Engineering - Department of Chemical Engineering and Food Engineering - Federal University of Santa Catarina (UFSC), Florianópolis, Brazil; [4]LAREX-Laboratory of Recycling, Waste Treatment and Extraction-Poli-USP, São Paulo, Brazil*

TP 676 **Novel Functional Proteomic Approach to Dissect G9a Interactomes Associated with Breast Tumorigenesis**; Adil Muneer[1]; Ling Xie[1]; Li Wang[1]; Jin Jian[2]; Xian Chen[1,3]; *[1]Department of Biochemistry & Biophysics, University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]Department of Pharmacological Sciences and Oncological Sciences, Icahn School of Medicine at Mount Sinai, New York City, NY; [3]Lineberger Comprehensive Cancer Center, University of North Carolina at Chapel Hill, Chapel Hill, NC*

TP 677 **Comparison and Optimization of Exosome Digestion and Fractionation Methods for Discovery Proteomic Analysis**; Elizabeth Nunn[1]; Nancy Sharkawy[1]; Amy-Joan L. Ham[1]; *[1]Belmont University, Nashville, TN*

TP 678 **Moving Towards Single-Cell Proteomics on a TIMS-qTOF Mass Spectrometer with PASEF**; Andreas-David Brunner[1]; Florian Meier[1]; Markus Lubeck[2]; Niels Goedecke[2]; Heiner Koch[2]; Scarlet Koch[2]; Oliver Raether[2]; Matthias Mann[1]; *[1]Max-Planck Institute of Biochemistry, Planegg, Germany; [2]Bruker Daltonik GmbH, Bremen, Germany*

TP 679 **Cysteine Directed Proteolysis for Middle Down Proteomics**; Joe R. Cannon[1]; J. Wade Harper[2]; Mark Cancilla[1]; *[1]Merck & Co., Inc., West Point, PA; [2]Harvard Medical School, Boston, MA*

TP 680 **Proteomic Characterization of RAS-Signaling**; German Monogarov[1]; Audrey Bettoun[2]; Yael Aylon[2]; Moshe Oren[2]; Jeroen Krijgsveld[1]; *[1]German Cancer Research Center (DKFZ), Heidelberg, Germany; [2]Weizmann Institute of Science, Rehovot, Israel*

TP 681 **Microflow DIA Using 15min Gradients Analyzes 40 Tumor Proteomes per Day and Effectively Detects Promising Protein Biomarkers**; Rui Sun[1]; Christie Hunter[2]; Chen Chen[3]; Huanhuan Gao[1]; Xue Cai[1]; Qiushi Zhang[1]; Bo Wang[4]; Xiaoyan Yu[5]; Xiaodong Teng[4]; Lirong Chen[6]; Ruedi Aebersold[6]; Yi Zhu[1]; Tiannan Guo[1]; *[1]School of Life Sciences, Westlake University, 18 Shilongshan Road, Hangzhou 310024, Zhejiang Province, China, Hang Zhou, China; [2]Sciex, Redwood City, CA; [3]Sciex, Shanghai, China; [4]Department of Pathology, The First Affiliated Hospital of College of Medicine, Zhejiang University, Hangzhou, China; [5]Department of Pathology, The Second Affiliated Hospital, Zhejiang University School of Medicine, Hangzhou, China; [6]Department of Biology, Institute of Molecular Systems Biology, ETH Zurich, Switzerland, Switzerland*

TP 682 **A Novel Strategy Enabled by a Photo-Cleavable Surfactant for Extracellular Matrix Proteomics**; Samantha J Knott[1]; Kyle Brown[1]; Bifan Chen[1]; Ying Ge[1,2,3]; *[1]The University of Wisconsin Madison's Department of Chemistry, Madison, WI; [2]The University of Wisconsin Madison's Department of Cell and Regenerative Biology, Madison, WI; [3]The University of Wisconsin Madison's Human Proteomics Training Program, Madison, WI*

TP 683 **Comprehensive Evaluation of Shotgun Proteomics Using Thermo Scientific Orbitrap Fusion Lumos Mass Spectrometer with FAIMS Pro Interface**; Yue Zhou[1]; Min Huang[1]; Xiangyun Yang[1]; Mo Hu[1]; Jing Li[1]; *[1]Thermo Fisher Scientific, Shanghai, China*

TP 684 **New Insights on Marfan Syndrome from Comparative N-Terminomics of Human Marfan and Non-Diseased Aortas**; Daniel Martin[1]; Frank Cikach[1]; Emidio Germano[1]; Eric Roselli[1]; Suneel Apte[1]; *[1]Cleveland Clinic, Cleveland, OH*

TP 685 **Enhancing the Isolation of DNA-Binding Protein from Yeast for High Confidence Interactome Analysis**; Ali Shariat-Panahi[1]; Aditya Mojumdar[1]; Jennifer A. Cobb[1]; David C. Schriemer[1]; *[1]Department of Biochemistry and Molecular Biology, University of Calgary, Calgary, AB*

TP 686 **Effects of Different Tissue Preserving Methods on Proteomic Results**; Ruiqi Jian[1]; Lihua Jiang[1]; Huaying Fang[1]; Meng Wang[1]; Joanne Chan[1]; Hua Tang[1]; Mike Snyder[1]; *[1]Stanford University School of Medicine, Palo Alto, CA*

TP 687 **Plasma Proteomics Goes High Throughput**; Raphael A Heilig[1]; Thomas Kosinski[2]; Yuxin Mi[3]; Katie L Burnham[3]; Julian C Knight[3]; Heiner Koch[2]; Roman Fischer[1]; *[1]Target Discovery Institute, Nuffield Department of Medicine, University of Oxford, Oxford, United Kingdom; [2]Bruker Daltonik GmbH, Bremen, Germany; [3]Wellcome Centre for Human Genetics, University of Oxford, Oxford, United Kingdom*

TP 688 **Large Scale Un-Depleted Human Serum Proteome Profiling and Targeted LC-MS/MS Evaluation toward Biomarker Discovery for Alzheimer's Disease**; Kaushik Kumar Dey[1]; Hong Wang[2]; Mingming Niu[2]; Xusheng Wang[2]; yuxin Li[2]; Ji-Hoon cho[2]; Haiyan Tan[2]; Ashutosh Mishra[2]; Anthony High[2]; Thomas G Beach[3]; Junmin Peng[2]; *[1]St Jude Children's Research Hospital, memphis, TN; [2]St Jude Children's Research Hospital, Memphis, TN; [3]Banner Sun Health Research Institute, Sun City, AZ*

TP 689 **The Ultra-Soft Picosecond-Infrared Laser - Multi-Tool for Sampling Tissues for Mass Spectrometric Omics**; Hartmut Schluter[1]; Marcel Kwiatkowski[2]; Marcus Wurlitzer[1]; Andrey Krutilin[1,3]; Frederik Busse[3]; Sascha Epp[3]; Nils-Owe Hansen[3]; Wesley Robertson[3,4]; Dwayne R.J. Miller[3]; *[1]UKE - Mass Spec Proteomics, Hamburg, Germany; [2]University of Groningen Faculty of Mathematics & Natural Sciences Pharmacokinetics, Toxicology and Targeting, Groningen, Netherlands; [3]Max Planck Institute for the Structure & Dynamics of Matter, Atomically Resolved*

Dynamics Division, Hamburg, Germany; [1]Georgia Institute of Technology, Georgia Tech Research Institute, Quantum Systems Division, Atlanta, GA 30318

TP 690 **A Novel, Small Molecule-Based Method for Tunable Cell-Surface Proximity Labeling to Enable Mapping of Immunomodulatory Receptor Protein Interactions**; Rob Oslund[1]; Niyi Fadeyi[1]; Tamara Reyes Robles[1]; Cory White[1]; Jake Tomlinson[1]; Kelly Crotty[1]; David H. Perlman[1]; Lee Roberts[1]; Grazia Piizzi[1]; Erik Hett[1]; *[1]Merck Exploratory Sciences Center, Cambridge, MA*

TP 691 **A Labeling Enrichment Method Based on Synergistic and Reversible Covalent Interactions for Seleno Protein Analysis**; Qingshi Meng[1]; Hongfu zhang[1]; Xiaohui feng[1]; *[1]Institute of Animal Sciences, CAAS, Beijing, China*

TP 692 **Enhancing the Sensitivity of Microflow-Based Bottom-Up Proteomic Analyses by the Post-Column Addition of Organic Solvent Modifiers**; Ute Distler[1]; Mateusz Krzysztof Łącki[1]; Markus Wanninger[2]; Stefan Tenzer[1]; *[1]University Medical Center Mainz, Mainz, Germany; [2]Waters Corporation, Milford, MA*

TP 693 **Combined Use of SAXS and LC-QTOF-MS in Structural Elucidation of Complex Biomolecules**; Hlengilizwe Nyoni[1]; Bhekie B. Mamba[1]; Titus TAM Msagati[1]; *[1]University of South Africa, Johannesburg, South Africa*

TP 694 **Utilizing Metabolic Isotope Labels to monitor protein and Lipid Metabolism to Integrate Alzheimer's Risk Factors into a Cohesive Model**; Joseph Creery[1]; Russell Denton[1]; Isabella James[1]; Kyle J Cutler[1]; John Price[2]; *[1]Brigham Young University, Provo, UT; [2]*, Provo, UT*

PROTEOMICS: QUANTITATIVE II
695-717

TP 695 **Understanding the Underlying Biological Pathways Affected by Treatment of Triple Negative Breast Cancer with Novel Natural Product Derivatives**; Alisha Birk[1]; Catherine C. Going[1]; Dhanir Tailor[2]; Vineet Kumar[2]; Abel Bermudez[1]; Fernando Garcia-Marqués[1]; Mallesh Pandrala[2]; Angel Resendez[2]; Meghan A. Rice[1]; Tanya Stoyanova[1, 3]; Sanjay V. Malhotra[1, 2, 3]; Sharon J. Pitteri[1, 3]; *[1]Department of Radiology, Canary Center at Stanford for Cancer Early Detection, Stanford University School of Medicine, Palo Alto, CA; [2]Department of Radiation Oncology, Stanford University School of Medicine, Palo Alto, CA; [3]Stanford Cancer Institute, Stanford University School of Medicine, Stanford, CA*

TP 696 **Block Design Enables Highly Reproducible Label-Free Quantitative Proteomics to Profile Cell Responses to Engineered Nanomaterials**; Tong Zhang[1]; Matthew J Gaffrey[1]; Becky M Hess[1]; Kari K Weitz[1]; Ronald J. Moore[1]; Brian D Thrall[1]; Wei-Jun Qian[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

TP 697 **Arc-Negative Extracellular Vesicles Promote Bidirectional Synaptic Communication through CaMKII**; Yi-Zhi Wang[1]; Samuel N. Smukowski[1]; Claire Piochon[1]; Ewa Bomba-warczak[1]; Qionger He[1]; Stacy A. Marshall[1]; Elizabeth T. Bartom[1]; Ali Shilatifard[1]; Anis Contractor[1]; Jeffrey N. Savas[1]; *[1]Northwestern University, Chicago, IL*

TP 698 **Multiplex TMT Based Protein Quantification on timsTOF Pro with Parallel Accumulation and Serial Fragmentation Method**; Pei Liu[1]; Brian P. Mooney[1]; Michael Sussman[2]; C. Michael Greenlief[1]; *[1]University of Missouri, Columbia, MO; [2]University of Wisconsin-Madison, Madison, WI*

TP 699 **Quantitative Proteomics: A New Tool for Understanding the Complexity of a Fermentation Media and the Upstream Process of Bacterial Vaccine**; Sébastien Peronin[1]; Julia Novion-Ducassou[1]; Thierry Eynard[1]; *[1]Sanofi Pasteur, Neuville-sur-Saône, France*

TP 700 **Dawn to Sunset Fasting for Four Weeks Has A Unique Proteomic Signature in Healthy Subjects**; Antrix Jain[1]; Sung Yun Jung[1]; Mustafa Abdulsada[1]; Antone Opekun[1]; Anna Malovannaya[1]; Prasun Jalal[1]; Ayse Mindikoglu[1]; *[1]Baylor College of Medicine, Houston, TX*

TP 701 **Determining and Characterizing Substrates of Impaired Protein Degradation in Models of Alzheimer's Disease**; Timothy Hark[1]; Ewa Bomba-Warczak[1]; Samuel N. Smukowski[1]; Laith Ali[1]; Jeffrey N. Savas[1]; *[1]Northwestern University, Chicago, IL*

TP 702 **Bayesian Confidence Intervals for Multiplexed Proteomics Integrate Ion Statistics with Peptide Quantification Concordance**; Leonid Peshkin[1]; Meera Gupta[2]; Lillia Ryazanova[2]; Martin Wuhr[2]; *[1]Harvard Medical School, Boston, MA; [2]Princeton University, Princeton, NJ*

TP 703 **A Super-Silac Method to Assess Myogenesis in Healthy vs Dystrophin-Deficient Muscle Cells**; Mansi V Goswami[1]; Emily Canessa[1]; Yetrib Hathout[1]; *[1]School of Pharmacy and pharmaceutical Sciences, University of Binghamton, Binghamton, NEW YORK*

TP 704 **Molecular Phenotypes Identification by Proteomic Profiling in Nemaline Myopathy Using timsTOF Pro Mass Spectrometer**; Liwen Zhang[1]; Sophie R. Harvey[1]; Rebecca A. Slick[2, 3, 4]; Jennifer A. Tinklenberg[2, 3, 4]; Federica Montanaro[5]; Michael W. Lawlor[2, 3]; *[1]The Ohio State University, Columbus, OH; [2]Department of Physiology, Medical College of Wisconsin,, Milwaukee, WI; [3]Division of Pediatric Pathology, Department of Pathology and Laboratory Medicine and Neuroscience Research Center Medical College of Wisconsin,, Milwaukee, WI; [4]Clinical and Translational Science Institute of Southeast Wisconsin, Medical College of Wisconsin,, Milwaukee, WI; [5]Institute of Child Health, University College London, London, United Kingdom*

TP 705 **Spatially-Resolved Neuroproteomics with IonStar Reveals Differential Landscapes of Signal Transduction Dysregulation in a Rat Ischemic Stroke Model**; Shichen Shen[1]; Min Ma[2]; Ming Zhang[1]; David Poulsen[1]; Jun Qu[1]; *[1]University at Buffalo, Buffalo, NY; [2]Roswell Park Comprehensive Cancer Center, Buffalo, NY*

TP 706 **Elucidating Novel Mechanisms of Action and Effects on Biological Pathways of Next Generation Anti-Cancer/ Bacteria Complexes Using UHR-MS/MS**; Kung Ching Cookson Chiu[1]; Yuko P. Y. Lam[1]; Christopher A. Wootton[1]; Hannah Bridgewater[1]; Feng Chen[1]; Mark P. Barrow[1]; John Moat[1]; Peter J. Sadler[1]; Peter B. O'Connor[1]; *[1]University of Warwick, Coventry, United Kingdom*

TP 707 **Insights into NEDD8 Inhibition on Proteostasis with Multiplexed Proteome Dynamics Profiling and super-Resolution Orbitrap Mass Spectrometry**; Nico Zinn[1]; Konstantin Aizikov[2]; Dmitry Grinfeld[2]; Arne Kreutzmann[2]; Daniel Mourad[2]; Oliver Lange[2]; Maria Fälth-Savitski[1]; Markus Queisser[3]; Alexander Makarov[2]; Marcus Bantscheff[1]; *[1]Cellzome, a GSK company, Heidelberg, Germany; [2]Thermo Fisher Scientific, Bremen, Germany; [3]GSK, Stevenage, United Kingdom*

TP 708 **Carrier Proteome Effect in Mass Spectrometry Based Approaches to Single Cell Proteomics**; Christopher M. Rose[1]; Atticus McCoy[1]; Donald S. Kirkpatrick[1]; *[1]Genentech, Inc., South San Francisco, CA*

TP 709 **Intact Glycopeptide Analysis of Triple Negative Breast Cancer Cell Lines Using IsoTaG**; Fernando Garcia-Marques[1]; Catherine C. Going[1]; Abel Bermudez[1]; Marc D Driessen[2]; Alisha Birk[1]; Carolyn R Bertozzi[2]; Christina Woo[3]; Sharon J. Pitteri[1]; *[1]Stanford University School of Medicine, Canary Center at Stanford for Cancer Early Detection, Palo Alto, CA; [2]Department of Chemistry and Howard Hughes Medical Institute, Stanford University, Stanford, CA; [3]Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA*

TP 710 **Isobaric Reporter Ion Cascades for High Capacity Multiplexing**; Brian Erickson[1]; Ryan Kunz[1]; Steven P Gygi[2]; Craig Braun[1]; *[1]IQ Proteomics LLC, Cambridge, MA; [2]Harvard Medical School, Boston, MA*

TP 711 **Detection of Peptide Level Changes in Cerebro Spinal Fluid Proteomes of Neurodegenerative Disease by Data-Independent Acquisition**; Deanna Plubell[1]; Eric Huang[1]; Michael S. Bereman[2]; Thomas Montine[3]; Michael J MacCoss[1]; *[1]University of Washington, Genome Sciences, Seattle, WA; [2]North Carolina State University, Raleigh, NC; [3]Stanford University, Stanford, CA*

TP 712 **Investigation and Characterization of the Jumping Translocation Breakpoint (JTB) Protein Using Mass Spectrometry Based Proteomics**; Madhuri Jayathirtha[1]; Devika Channaveerappa[1]; Kangning Li[1]; Costel C Darie[1]; *[1]Clarkson University, Potsdam, NY*

TP 713 **Effects to the Human Proteome Due to Legacy Chemical Exposure in the Great Lakes**; Emmalyn J Dupree[1]; Bernard Crimmins[1]; Thomas Holsen[1]; James Pagano[2]; Brooke Thompson[3]; Krista Christensen[3]; Michelle Raymond[3]; Jon Meiman[3]; Costel C Darie[1]; *[1]Clarkson University, Potsdam, NY; [2]SUNY Oswego, Oswego, NY; [3]Wisconsin Department of Health Services, Madison, WI*

TP 714 **High-Throughput Quantitative Profiling of Small GTPases in Brain Tissues of Alzheimer's Disease Patients**; Ming Huang[1]; Yinsheng Wang[2]; *[1]University of California, Riverside, CA; [2]University of California, Riverside, Riverside, CA*

TP 715 **Discovery of Novel Guanine-Quadruplex-Unwinding Proteins**; Zi Gao[1]; Lin Li[1]; Preston Williams[1]; Yinsheng Wang[1]; *[1]University of California, Riverside, Riverside, CA*

TP 716 **Quantitative Profiling of Small GTPases in Secretome of Cultured Human Cancer Cells Using Scheduled MRM Coupled with Stable Isotope-Labeled Peptides**; Tianyu Qi[1]; Ming Huang[1]; Yinsheng Wang[1]; *[1]UC Riverside, Riverside, CA*

TP 717 **Proteome Quality Control Addressing Qualitative and Quantitative Needs for Trapped Ion Mobility Spectrometry and Parallel Accumulation Serial Fragmentation**; Michael Krawitzky[1]; Chris Adams[1]; Conor Mullens[2]; Shourjo Ghose[2]; Matthew Willetts[2]; Gary Kruppa[2]; *[1]Bruker Daltonics Inc., San Jose, CA; [2]Bruker Daltonics Inc., Billerica, MA*

PROTEOMICS: TOP DOWN ANALYSIS II
718-737

TP 718 **Proteoform Family Identification and Quantification Using Proteoform Suite**; Leah V Schaffer[1]; Michael R Shortreed[1]; Anthony J Cesnik[1]; Jarred W Rensvold[2]; Adam Jochem[2]; Trisha Tucholski[1]; Mark Scalf[1]; Brian L Frey[1]; Ying Ge[1]; David J Pagliarini[1,2]; Lloyd M Smith[1]; *[1]University of Wisconsin - Madison, Madison, WI; [2]Morgridge Institute for Research, Madison, WI*

TP 719 **An Iodine-Based N-Terminal Mass Defect Labelling Strategy for Improved *de novo* Top-Down Protein Sequencing**; Lavrentis Dimitrios Galanopoulos[1]; Lennete Kjaer[1]; Adam Karpinski[2]; Sam Hughes[1]; David J Clarke[1]; *[1]University of Edinburgh, Edinburgh, United Kingdom; [2]University of Warsaw, Warsaw, Poland*

TP 720 **FLASHDeconv: Ultra-Fast High-Quality Deconvolution Enables Online Processing of Top-Down MS Data**; Kyowon Jeong[1]; Jihyung Kim[1]; Manasi Gaikwad[2]; Siti Nurul Hidayah[2]; Hartmut Schlüter[2]; Oliver Kohlbacher[1,3,4,5,6]; *[1]Applied Bioinformatics, Department for Computer Science, University of Tübingen, Tübingen, Germany; [2]Mass Spectrometric Proteomics, Institute of Clinical Chemistry and Laboratory Medicine, Campus Forschung, Universitätsklinikum Hamburg-Eppendorf, Hamburg, Germany; [3]Center for Bioinformatics, University of Tübingen, Tübingen, Germany; [4]Center for Quantitative Biology, University of Tübingen, Tübingen, Germany; [5]Biomolecular Interactions, Max Planck Institute for Developmental Biology, Tübingen, Germany; [6]Translational Bioinformatics, University Hospital Tübingen, Tübingen, Germany*

TP 721 **Isotope Pattern Matching Software for Mass Analysis of Intact Proteins**; Greg T. Blakney[1]; Lissa C Anderson[1]; Allen G. Marshall[1]; Christopher L. Hendrickson[1,2]; *[1]National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL; [2]Florida State University, Tallahassee, FL*

TP 722 **A Fast and High-Throughput Sample Preparation Platform Coupled with Top-Down Mass Spectrometry for Therapeutic Antibody Analysis**; Hae-Min Park[1]; Jared Drader[2]; Valerie J. Winton[1]; Sheri Manalili-Wheeler[2]; Neil L. Kelleher[1]; Philip D. Compton[2]; *[1]Northwestern University, Evanston, IL; [2]Integrated Protein Technologies, Inc., Evanston, IL*

TP 723 **Comprehensive Characterization of Kinases by Top-Down Mass Spectrometry**; Zhijie Wu[1]; Yutong Jin[1]; Bifan Chen[1]; Ying Ge[1]; *[1]University of Wisconsin, Madison, Madison, WI*

TP 724 **Early Diagnostics of Clinical Samples by Top-Down Proteomics Using Capillary Electrophoresis-Electrospray Ionization-Mass Spectrometry (CESI-MS)**; Amir Prior[1]; David Morgenstern[1]; Alexandra Gabashvili[1]; Dalia Elinger[1]; Hila Wolf-Levy[1]; Moshe E. Gatt[2]; Yishai Levin[1]; *[1]Weizmann Institute of Science, Rehovot, Israel; [2]Hadassah-Hebrew University Medical School, Jerusalem, Israel*

TP 725 **High-Throughput Top-Down FAIMS Data Analysis with ProSight PD Nodes in the Thermo Scientific Proteome Discoverer Software**; Susan E. Abbatiello[1]; Michael W. Belford[2]; Philip D. Compton[3]; Kenneth R. Durbin[4]; Ryan Fellers[4]; Vincent Gerbasi[3]; Joseph Greer[4]; Mick Greer[6]; David Horn[2]; Romain Huguet[2]; Neil L Kelleher[3]; Richard LeDuc[4]; Scott M. Peterman[2]; Paul M Thomas[3]; *[1]Northeastern University, Boston, MA; [2]Thermo Fisher Scientific, San Jose, CA; [3]Northwestern University, Evanston, IL; [4]Proteinaceous, Inc., Evanston, IL; [5]Thermo Fisher Scientific, Austin, TX*

TP 726 **Proteomic Characterization of Truncated Proteoforms in MDSC Extracellular Vesicles**; Dapeng Chen[1]; Fabio P Gomes[1]; Suzanne Ostrand-Rosenberg[2]; Catherine Fenselau[1]; *[1]Department of Chemistry and Biochemistry, University of Maryland, College Park, MD; [2]Department of Biological Sciences, University of Maryland Baltimore County, Baltimore, MD*

TP 727 **Top Down Quantitation of Oxidative Proteomics**; Surendar Tadi[1]; Joshua S Sharp[2]; *[1]University of Mississippi, Oxford, MS; [2]University of Mississippi, University, MS*

TP 728 **Native State Chemical Tagging Approaches for the Free Radical-Initiated Sequencing of Intact Protein Complexes**; Carolina Rojas Ramirez[1]; Daniel A. Polasky[1]; Brandon T. Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI*

TP 729 **Direct Thermal Proteome Profiling Using Quantitative Top-Down Proteomics**; Kellye A Cupp-Sutton[1]; Zhe Wang[1]; Si Wu[1]; *[1]University of Oklahoma, Norman*

TP 730 **MASH Explorer, a Universal, Comprehensive, and User-Friendly Software Environment for Top-down Proteomics**; Sean J McIlwain[1]; Zhijie Wu[2]; Kent Wenger[3]; Molly Wetzel[3]; Trisha Tucholski[2]; Xiaowen Liu[4,5]; Ruixiang Sun[6]; Irene M Ong[1,7]; Ying Ge[2,3,8,9]; *[1]Department of Biostatistics and Medical Informatics, University of Wisconsin, Madison, WI; [2]Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706; [3]Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; [4]Department of BioHealth Informatics, Indiana University-Purdue*

University Indianapolis, Indianapolis, Indiana; [5]Center for Computational Biology and Bioinformatics, Indiana University School of Medicine, Indianapolis, Indiana; [6]Institute of Computing Technology, CAS, Beijing, China; [7]Department of Obstetrics and Gynecology, University of Wisconsin-Madison, Madison, WI; [8]Molecular and Cellular Pharmacology Program, University of Wisconsin, Madison, WI; [9]Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI

TP 731 **Comparison of ECD versus ETD for Low-Charge State Proteins in Orbitrap and Q-ToF Instruments**; Yury V. Vasil'ev[1,2]; Jared B. Shaw[3]; Valery G. Voinov[1,4]; Joseph C. Meeuwsen[5]; Nathan I. Lopez[1,2]; Joseph S. Beckman[2,6]; *[1]Linus Pauling Institute, Oregon State University, Corvallis, OR; [2]e-MSion, Inc., Corvallis, OR; [3]Pacific Northwest National Laboratory, Richland, WA; [4]e-Msion Inc., Corvallis, OR; [5]Oregon State University, Crovalis, OR; [6]Linus Pauling Institute, Oregon State University,, Corvallis, OR*

TP 732 **Targeting a Subset of the Membrane Proteome for Top-Down Mass Spectrometry; the Proteolipids that Extract into Chloroform**; Whitaker Cohn[1]; Lucy Gao[1]; Julian Whitelegge[1]; *[1]University of California LA, Los Angeles, CA*

TP 733 **Deep Intact Proteome Quantification Using Protein-Level Tandem Mass Tag (TMT) Labeling and Online 2D Liquid Chromatography**; Dahang Yu[1]; Zhe Wang[1]; Kellye A Cupp-Sutton[1]; Kenneth Smith[2]; Xiaowen Liu[3]; Si Wu[1]; *[1]University of Oklahoma, Norman, OK; [2]Oklahoma Medical Research Foundation, Oklahoma City, OK; [3]Indiana University-Purdue University Indianapolis, Indianapolis, IN*

TP 734 **Investigating the Stability of Linear Polyacrylamide Coating for Capillary Zone Electrophoresis-Tandem Mass Spectrometry-Based Top-Down Proteomics**; Tian Xu; *Michigan State University, East Lansing, MI*

TP 735 **Top-Down Proteomics in Support of the Industrial Milk Production Process**; Catherine Rawlins[1,2]; Stéphane Claverol[2]; Audrey Romelard[3]; Caroline Tokarski[1,2]; *[1]Institute of Chemistry and Biology of Membrane and NanoObjects, UMR CNRS 5248, Bordeaux, France; [2]Proteome Platform, Center of Functional Genomics of Bordeaux, University of Bordeaux, Bordeaux, France; [3]Ingredia Dairy Experts, Arras, France*

TP 736 **Investigating the Protein Recovery of Membrane-Based Sample Preparation Methods for Top-Down Proteomics**; Qianjie Wang; *Michigan State University, East Lansing, MI*

TP 737 **Top-Down Analysis of Snake Venom Proteoforms through *de novo* Sequencing**; Kira Vyatkina[1]; Daniel Petras[2]; *[1]SPb Academic University, St Petersburg, Russian Federation; [2]University of California, San Diego, CA*

SMALL MOLECULES: QUALITATIVE ANALYSIS
738-756

TP 738 **Interpretation of Mass Spectrometric Data for Structure Elucidation of a New Endogenous Organosulfur Metabolite**; Qibo Zhang[1]; Lisa A. Ford[1]; Anne M. Evans[1]; Douglas R. Toal[1]; *[1]Metabolon, Morrisville, NC*

TP 739 **Mass Spectroscopic Analysis of Phenol Derivatives by Gibbs Reaction**; Sabyasachy Mistry; *Purdue University, West Lafayette*

TP 740 **An Efficient Approach to Oligomer Screening of Extractables Samples Using Liquid Chromatography Quadrupole Time-of-flight Mass Spectrometry (LC/Q-TOF)**; Kuang-Wei Yang[1]; Jin Ren[1]; Benben Song[1]; *[1]Pall Corporation, Westborough, MA*

TP 741 **Pharmaceutical Degradation Product Profiling on an Orbitrap ID-X Tribrid Mass Spectrometry Platform**; G. Charles Cheng[1]; Kate J. Comstock[2]; Xiaojie C. Ding[2]; Seema Sharma[2]; *[1]Blueprint Medicines, Cambridge, MA; [2]Thermo Fisher Scientific, San Jose, CA*

TP 742 **Investigation and Profiling of Organic Solvent Based Lithium Ion Battery Electrolytes and the Decomposition Products**; Nan Hu; *Agilent Technologies, Beijing, China*

TP 743 **An Alternative Screening Protocol for Determining Amines in Industrial Materials Using Combined Flow Injection (FI) Electrospray-TOFMS and Electrospray-TOFMS/MS Methods**; Dale A. Willcox[1]; Jenan M. Elias[2]; Kelli Magarelli[1]; Marshall Henry[1]; *[1]Intertek Allentown, Allentown, PA; [2]Intertek, Allentown, PA*

TP 744 **Identification of Degradation Products of Epirubicin Based on multiple heart-cut2D LC-Q TOF**; Yaping Zhang[1]; Hui Ouyang[2]; Congfang Lai[3]; *[1]Agilent Technologies, Shanghai, China; [2]Jiangxi University of Traditional Chinese Medicine, Nanchang, China; [3]Agilent Technologies(China) Co. Ltd., Beijing, China*

TP 745 **Elucidating Disperse Dye Photodegradation Pathways Using Tandem Mass Spectrometry and Density Functional Theory**; Ciera E Cipriani[1]; Erol Yildirim[2]; Cody P Zane[1]; Stephanie E Atkinson[1]; Nelson R Vinueza[1]; Melissa A Pasquinelli[1]; *[1]Wilson College of Textiles, North Carolina State University, Raleigh, NC; [2]Institute of High Performance Computing, Agency for Science, Technology and Research, Singapore*

TP 746 **Simplified Approach for Structural Elucidation and Quantitation for Pharmaceutical API and Related Impurities Using Q-TOF**; Purushottam Janardan Sutar[1]; Shailendra Rane[1]; Shailesh Damale[1]; Rashi Kochhar[1]; Deepti Bhandarkar[1]; Anant Lohar[1]; Ashutosh Shelar[1]; Bhaumik Trivedi[1]; Navin Devadiga[1]; Ajit Datar[1]; Pratap Rasam[1]; Jitendra Kelkar[1]; *[1]Shimadzu Analytical (India) Pvt. Ltd., Mumbai, India*

TP 747 **So Which Is It? In-Column Thermal Isomerization of Volatile Acid Emitted from Urethane Conformal Coating and Determining Identification Confidence**; Curtis D. Mowry[1]; Lance L. Miller[1]; Jessica Roman[1]; Adam S. Pimentel[1]; Raymond Fuentes[1]; Jason R. Brown[1]; *[1]Sandia National Laboratories, Albuquerque, NM*

TP 748 **Development of LC-MS/MS Method to Detect and Evaluate Clinically Relevant Antibiotics in Human Stool Samples from Patients with Cholera**; Laura Bailey[1]; Ashton Marrazzo[1]; Manasi Kamat[1]; Eric J. Nelson[1]; Kari B. Green[1]; *[1]University of Florida, Gainesville, FL*

TP 749 **Improved Structural Characterisation of Molecules with a Chimeric Collision Cell with both Electron-Based and Collision-Induced Dissociation Capability**; Yves Le blanc[1]; Takashi Baba[2]; Pavel Ryumin[2]; Bill Loyd[2]; Eva Duchoslav[2]; *[1]SCIEX, Concord, On, ON; [2]SCIEX, Concord, ON*

TP 750 **Detection of Reactive Dye from soil *via* QuEChERS extraction and Quadrupole Time-Of-Flight Mass Spectrometry**; Xinyi Sui[1]; Chengcheng Feng[1]; Yufei Chen[2]; Mary Ankeny[3]; Nelson Vinueza[1]; *[1]North Carolina State University, Raleigh, NC; [2]Jordi Labs, Mansfield, MA; [3]Cotton Incorporated., Cary, NC*

TP 751 **Application of Mass Spectrometry for Studying the Degradation of Amino Acids and Volatile Organic Compounds by Chlorine Dioxide**; Ngee Sing Chong[1]; Abdul Hoque[1,2]; Heather Deal[1]; Beng Guat Ooi[1]; *[1]Middle Tennessee State University, Murfreesboro, TN; [2]University of Cincinnati, Cincinnati , OH*

TP 752 **Identification of Impurities in the Organic Solvents Used in the Semiconductor Field by Using GC-HRTOFMS with EI/FI**; Koji Okuda[1]; John Dane[1]; Robert Cody[1]; *[1]JEOL USA, Inc., Peabody, MA*

TP 753 **Selective Gas-Phase Mass Tagging *via* Ion/Molecule Reactions Combined with Single Analyzer Neutral Loss Scans to Probe Pharmaceutical Mixtures**; Dalton T. Snyder[1]; Lucas J. Szalwinski[1]; Alice Pilo[2]; Nina K. Jarrah[2]; R. Graham Cooks[1]; *[1]Purdue University, West Lafayette, IN; [2]Merck & Co., Inc., Rahway, NJ*

TP 754 **Evaluation of Alternate MS/MS Fragmentation Tools, Including UVPD and EID, for the Structural Elucidation of Trace Level Metabolites**; Jeffrey Gilbert[1]; Jesse L Balcer[1]; David G McCaskill[1]; Nick N Wang[1]; Chengli C Zu[1]; Yelena A Adelfinskaya[1]; J.C. Yves Le blanc[2]; *[1]Corteva Agriscience, Indianapolis, IN; [2]SCIEX, Concord, ON*

TP 755 **A New Electrochemical Route for Carbon-Carbon Bond Formation: Electrochemistry-Assisted Intermolecular [3+2] Annulation of N-cyclopropyl-3, 5-dimethylaniline and Styrene**; Qi Wang[1]; Qile Wang[2]; Nan Zheng[2]; Richard N Zare[3]; Yuexiang Zhang[4]; Hao Chen[1,4]; *[1]New Jersey Institute of Technology, Newark, NJ; [2]University of Arkansas, Fayetteville, AR; [3]Stanford University, Stanford, CA; [4]Ohio University, Athens, OH*

TP 756 **Building Local Proprietary Libraries with Automated MSn Spectral Tree Curation and New Library Searching Tools**; Xiaojie C. Ding[1]; Kate J. Comstock[2]; Seema Sharma[2]; Mark Sanders[2]; Michal Raab[3]; *[1]Thermo Scientific, San Jose, Ca, CA; [2]Thermo Fisher Scientific, San Jose, CA; [3]HighChem, Bratislava, Slovakia*

SYSTEMS BIOLOGY
757-780

TP 757 **Molar Quantification of Metabolic Pathways Elucidates the Mechanism of Metabolic Shift In *Caenorhabditis elegans***; Bharath Kumar Raghuraman[1]; Sider Penkov[1]; Teymuras V. Kurzchalia[1]; Andrej Shevchenko[1]; *[1]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany*

TP 758 **Using Highly-Multiplexed Panels of Quantitative MRM Assays to Establish Normal Tissue Protein Concentrations in Mice**; Sarah Michaud[1]; Helena Pětrošová[1]; Angela Jackson[1]; Andrea L. Palmer[1]; Nicholas J. T. Sinclair[1]; Ann Flenniken[2,3]; Lauryl Nutter[2,4]; Colin McKerlie[2,4]; Milan Ganguly[2,4]; Ingo Feldmann[5]; Olga Shevchuk[5]; Yassene Mohammed[1,6]; David Schibli[1]; Albert Sickmann[5]; Christoph H. Borchers[1,7,8,9]; *[1]University of Victoria-Genome BC Proteomics Centre, Victoria, BC; [2]The Centre for Phenogenomics, Toronto, ON; [3]Lunenfeld-Tanenbaum Research Institute, Sinai Health System, Toronto, ON; [4]The Hospital for Sick Children, Toronto, ON; [5]Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany; [6]Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; [7]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; [8]Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; [9]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC*

TP 759 **Interferon Stimulated Gene 15 Controls Phagosome Maturation**; Frederic Lamoliatte[1]; Tiaan Heunis[1]; Anetta Svitorka Hartlova[1]; Matthias Trost[1]; *[1]ICAMB, Newcastle University, Newcastle Upon Tyne, United Kingdom*

TP 760 **Multi-Omics Profiling and Customized gRNA Library CRISPR-CAS9 Genomic Screening Identify Cancer Vulnerabilities in Brain Tumors**; Hong Wang[1]; Mingming Niu[2]; Timothy I. Shaw[2]; yuxin Li[2]; Ji-Hoon cho[2]; Anthony High[1]; Vishwajeeth Pagala[2]; Xusheng Wang[2]; Junmin Peng[1]; *[1]St. Jude Children's Research Hospital, Memphis, TN; [2]St.Jude children's Research hospi, Memphis, TN*

TP 761 **Longitudinal Metaproteomic Characterization Simultaneously Reveals the Presence and Functions of Bacteria and Eukaryotes in the Gut Microbiomes of Preterm Infants**; Samantha L. Peters[1,2]; Patrick T. West[3]; Feiqiao Brian Yu[4]; Brian A. Firek[5]; Michael J. Morowitz[5]; Jillian F. Banfield[6]; Robert L. Hettich[2,7]; *[1]Oak Ridge National Laboratory, Oak Ridge, Tennessee; [2]University of Tennessee, Knoxville, TN; [3]University of California Berkeley, Berkeley, California; [4]Chan Zuckerberg Biohub, San Francisco, CA; [5]University of Pittsburgh School of Medicine, Pittsburgh, PA; [6]University of California, Berkley, Berkeley, CA; [7]Oak Ridge National Laboratory, Oak Ridge, TN*

TP 762 **Advancing Insights in Molecular Regulation of *Leishmania donovani* by Integration of Multi-Omics Data.**; Bart Cuypers[1,2]; Malgorzata A. Domagalska[2]; Pieter Meysman[1]; Wout Bittremieux[1,3]; Hideo Imamura[2]; Dirk Valkenborg[4]; Geert Baggerman[1,5]; Inge Mertens[1,5]; Jean-Claude Dujardin[1,2]; Kris Laukens[1]; *[1]University Of Antwerp, Antwerp, Belgium; [2]Institute Of Tropical Medicine, Antwerp, Belgium; [3]University of Washington, Seattle, WA; [4]University of Hasselt, Diepenbeek, Belgium; [5]Vito, Mol, Belgium*

TP 763 **A Novel HLA-Peptide Profiling Workflow Called MAPTAC (Mono-Allelic-Purification-with-Tagged-Allele-Constructs) Leverages Mass Spectrometry to Improve Neoantigen Prediction**; Daniel Rothenberg[1]; Jennifer Abelin[1]; Dominik Barthelme[1]; Rob C Oslund[1]; Amanda L Creech[1]; Tyler Colson[1]; Scott P Goulding[1]; Lia R Serrano[1]; Chris Mcgann[1]; Ying S Ting[1]; Yusuf Nasrullah[1]; Janani Sridar[1]; Dewi Harjanto[1]; Matt Malloy[1]; Christina Kuksin[1]; Joel Greshock[1]; Terri A Addona[1]; Michael S Rooney[1]; *[1]Neon Therapeutics, Cambridge, MA*

TP 764 **MS-Based Metaproteomics Reveals Details of Microbiome Adaptation to Increasing Plant Biomass Substrate Loading to Maintain Undiminished Lignocellulose Solubilization**; Payal Chirania[1,2]; Suresh Poudel[2]; Richard J. Giannone[1,2]; Xiaoyu Liang[3]; Evert K. Holwerda[3]; Lee R. Lynd[3]; Robert L. Hettich[1,2]; *[1]University of Tennessee, Knoxville, Knoxville, TN; [2]Oak Ridge National Laboratory, Oak Ridge, TN; [3]Dartmouth College, Hanover, NH*

TP 765 **Identifying Novel TBK1 Substrates Using an Optimized TMT-Based Phosphoproteomics Method**; Laura E Herring[1]; Emily M Wilkerson[1]; Lianxin Hu[1]; Dennis Goldfarb[1]; Lee M Graves[1]; Qing Zhang[1]; *[1]UNC-Chapel Hill, Chapel Hill, NC*

TP 766 **Metagenomic-based Metaproteomic Functional Characterization of the Sargasso Sea in a Three Year Time Series Dataset**; Mak Saito[1]; Brian Searle[2]; Dawn Moran[3]; Jaci Saunders[3]; Noelle Held[3]; Chris Dupont[4]; Rod Johnson[5]; Matthew McIlvin[3]; *[1]Woods Hole Oceanographic Inst., Woods Hole Ma 02543, MA; [2]Institute for Systems Biology, Seattle, Washington; [3]Woods Hole Oceanographic Institution, Woods Hole; [4]J. Craig Venter Institute, La Jolla, CA; [5]Bermuda Institute of Ocean Sciences, St. Georges, Bermuda*

TP 767 **Single Colony Metaproteomes of a Marine Bacterium: Exploring Heterogeneity in the Natural Environment**; Noelle Held[1,2]; Matthew McIlvin[1]; Eric Webb[3]; Mak Saito[1]; *[1]Woods Hole Oceanographic Institution, Woods Hole; [2]Massachusetts Institute of Technology, Cambridge, MA; [3]University of Southern California, Los Angeles, CA*

TP 768 **Cellular Dynamics of Protein-Protein Interactions Mediated by Serine Phosphorylation**; Kyle Mohler[1]; Karl Barber[1]; Jack Moen[1]; Svetlana Rogulina[1]; Jesse Rinehart[1]; *[1]Yale University, West Haven, CT*

TP 769 **Quantitative Protein Expression and Phosphorylation Level Profiling Using 11-plex TMT Reagents: Application to 110 Yeast Kinase and Phosphatase Deletion Strains**; Jiaming Li[1]; Joao A. Paulo[1]; David Nusinow[1]; Edward Huttlin[1]; Steven Gygi[1]; *[1]Harvard Medical School, Boston, MA*

TP 770 **Targeted Proteomics-Driven Computational Modeling of the Mouse Macrophage Toll-like Receptor Signaling Pathway**; Nathan P Manes[1]; Jessica M Calzola[1]; Pauline R Kaplan[1]; Iain DC Fraser[1]; Ronald N Germain[1]; Martin Meier-Schellersheim[1]; Aleksandra Nita-lazar[1]; *[1]National Institutes of Health, Bethesda, MD*

TP 771 **Universal Proteomic Approach of Capturing Novel and Dynamic Trafficking Organelle Assemblies**; Nan Wang[1]; Thomas Lee[1]; Mary Katherine Connacher[1]; Tianjing Hu[1]; Scott Stuart[1]; Natalie Ahn[1]; *[1]Department of Biochemistry, University of Colorado, Boulder, CO*

TP 772 **Investigating Proteome Changes Caused by ABCA7 Missense Variants that Confer Alzheimer's Disease Risk in African Americans**; Tyra M. Avery[1]; Kaitlyn E. Stepler[1]; Prem Prakash[2]; Jamaine S. Davis[2]; Renã A.S. Robinson[1,3,4,5,6]; *[1]Vanderbilt University Department of Chemistry, Nashville, TN; [2]Meharry Medical College Department of Biochemistry and Cancer Biology, Nashville, TN; [3]Vanderbilt University Medical Center Department of Neurology, Nashville, TN; [4]Vanderbilt Memory and Alzheimer's Center Vanderbilt University Medical Center, Nashville, TN; [5]Vanderbilt Institute of Chemical Biology, Nashville, TN; [6]Vanderbilt Brain Institute, Nashville, TN*

TP 773 **A Peptidogenomics Approach Reveals the Identification of the *Canidae hepcidin***; Martin K Mead[1]; Melissa Claus[2,3]; Ed Litton[4,5]; Lisa Smart[2,3]; Anthea Raisis[2,3]; Gabriele Rossi[2,3]; Robert D Trengove[1,6]; Joel P. A. Gummer[1,6]; *[1]Separation Science and Metabolomics Laboratory, Research and Innovation, Murdoch University, Perth, Australia; [2]College of Veterinary Medicine, Murdoch University, Perth, Australia; [3]School of Veterinary Science, Murdoch University, Perth, Australia; [4]Intensive Care Unit, Fiona Stanley Hospital, Perth, Australia; [5]School of Medicine, University of Western Australia, Perth, Australia; [6]Metabolomics Australia, Western Australia Node, Murdoch University, Perth, Australia*

TP 774 **Proteome-Wide Optimization of Orthogonal Translation Systems**; Jack M Moen[1]; Kyle Mohler[1]; Svetlana Rogulina[1]; Jesse Rinehart[1]; *[1]Yale University, West Haven, CT*

TP 775 **Proteotyping 30 Mouse Knockouts Using Targeted Quantitative Plasma Proteomics with Heavy-Labeled Internal Standards and the Software Tool KOPF Gene**; Yassene Mohammed[1,2]; Simon Roome[1]; Sarah A. Michaud[1]; Helena Pětrošová[1]; Ann Flenniken[3,4]; Lauryl Nutter[3,5]; Colin McKerlie[3,5]; Milan Ganguly[3,5]; Christoph H. Borchers[1,6,7,8]; *[1]University of Victoria-Genome BC Proteomics Centre, Victoria, BC; [2]Center for Proteomics and Metabolomics, Leiden University Medical Center, Leiden, Netherlands; [3]The Centre for Phenogenomics, Toronto, ON; [4]Lunenfeld-Tanenbaum Research Institute, Sinai Health System, Toronto, ON; [5]The Hospital for Sick Children, Toronto, ON; [6]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; [7]Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; [8]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC*

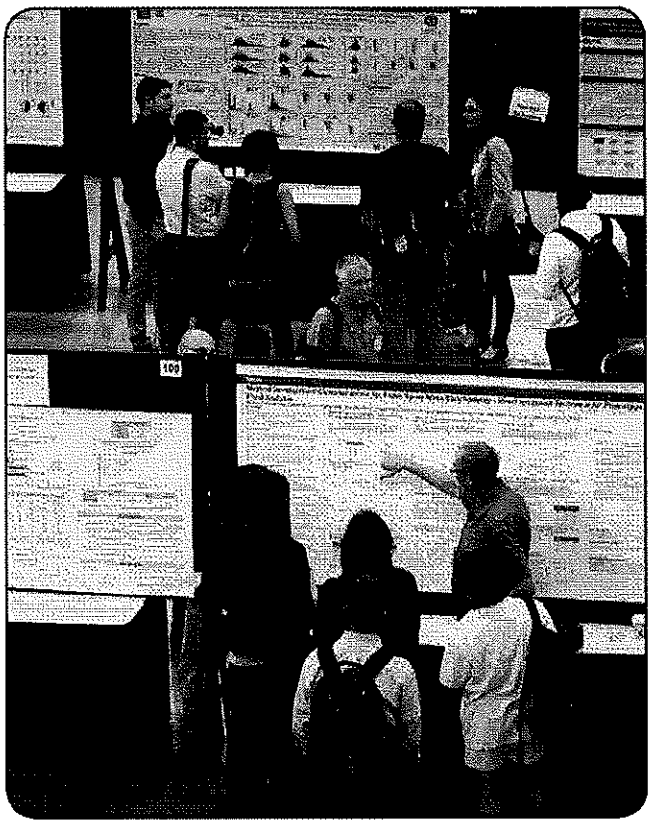
TP 776 **Top-down Proteomics for Deciphering Hypertrophic Cardiomyopathy in a Patient-Specific Engineered Cardiac Tissue Disease Model**; Stanford D. Mitchell[1,2]; Willem J. de Lange[3]; Jianhua Zhang[4]; Gina Kim[4]; Trisha Tucholski[5]; Timothy J. Kamp[1,4]; J. Carter Ralphe[3]; Ying Ge[1,2,5]; *[1]Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; [2]Molecular and Cellular Pharmacology Graduate Training Program, Madison, Wisconsin; [3]Department of Pediatrics, School of Medicine and Public Health, University of Wisconsin-Madison, MADISON, WI; [4]Department of Medicine, School of Medicine and Public Health, University of Wisconsin - Madison, Madison, Wisconsin; [5]Department of Chemistry, University of Wisconsin-Madison, Madison, WI*

TP 777 **Quantitative Lipidomics and Proteomics Analsyis of HDL Particles from Patient Samples Separated by Preparative Two Dimensional Gel Electrophoresis**; Zsuzsanna Kuklenyik[1]; Katrin Niisuke[2]; Michael Gardner[1]; Antony Lehtikoski[1]; Christopher Toth[1]; John R Barr[1]; Tomas Vaisar[3,4]; Bela Asztalos[2]; *[1]Centers for Disease Control and Prevention, Atlanta, Georgia; [2]Tufts University, Boston, MA; [3]University of Washington, DEOHS, Seattle, WA; [4]University of Washington, UWMDI, Seattle, WA*

TP 778 **A Proteogenomic Systems Analysis Reveals Alterations in RNA Binding Proteins and RNA Splicing in Alzheimer's Disease Brain**; Erik C.B. Johnson[1]; Eric B. Dammer[1]; Duc M. Duong[1]; Luming Yin[1]; Madhav Thambisetty[2]; Juan C. Troncoso[3]; James J. Lah[1]; Allan I. Levey[1]; Nicholas T. Seyfried[1]; *[1]Emory University, Atlanta, GA; [2]National Institute on Aging, National Institutes of Health, Baltimore, MD; [3]Johns Hopkins University School of Medicine, Baltimore, MD*

TP 779 **Systematic AP/MS and Genetic Interaction Mapping of the Ras Pathway Reveals New Effectors and Vulnerabilities**; Peter K Jackson[1]; Marcus R Kelly[1]; Kaja Kostyrko[2]; Kyuho Han[1]; Michael Bassik[1]; Alejandro Sweet-Cordero[2]; *[1]Stanford University School of Medicine, Stanford, CA; [2]UCSF, San Francisco, CA*

TP 780 **Integrated Proteome and Phosphoproteome Analysis Suggest a Role of JNK3 in Myelination and Synaptic Function**; Jan-Philip Schülke[1]; Mercedes Priego Luque[2]; Norma Hernandez[2]; Daniel Bader[1]; Barbara Kracher[1]; Sarah Elschenbroich[1]; Uli Ohmayer[1]; Oxana Lavrova[3]; Jim Rosinski[4]; Christoph Schaab[1]; Gerardo A Morfini[2]; Ignacio Munoz-Sanjuan[3]; *[1]Evotec (München) GmbH, Martinsried, Germany; [2]University of Illinois at Chicago, Department of Anatomy and Cell Biology, Chicago, IL; [3]CHDI Foundation, Los Angeles, CA; [4]CHDI Foundation, Princeton, NJ*



Set up all Wednesday posters
7:00 - 8:00 am
Odd-numbered posters present
10:30 - 11:30 am PLUS 12:30 – 2:30 pm
Even-numbered posters present
10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm
Remove all Wednesday posters
7:00 - 8:00 pm

Ambient Ionization: Applications I 001-031
Antibodies & Antibody Drug Conjugates II 032-064
Biomarkers: Discovery II 065-095
Biomarkers: Quantitative Analysis III 096-126
Biomolecular Structure Analysis: Chemical Crosslinking and Covalent Labeling II 127-153
Cannabis 154-179
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Imaging MS: Disease Markers I 361-379
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WP 002 **Open Ambient Ionisation Source Coupled to a Mass Detector for Rapid Detection of Undeclared Active Ingredient(s) in Online Health Supplements**; Chris Henry; *Waters Corportaion, Cheshire, United Kingdom*

WP 003 **Protein Screening of Native Brain Sections Using LESA-TIMS-MS**; Yarixa L. Cintron-Diaz[1]; Mario E. Gomez Hernandez[1]; Jennifer Dziedzic[1]; Tomas R. Guilarte[1]; Francisco A. Fernandez-Lima[1]; *[1]Florida International University, Miami, FL*

WP 004 **Absolute Quantitation of Tryptophan Metabolites in Brain Tissue Using Paper Spray Ionization-High Resolution Mass Spectrometry**; Richard C Dilworth[1]; Vanessa Y. Rubio[1]; Gary P Wang[1]; Timothy J. Garrett[1]; *[1]University of Florida, Gainesville, FL*

WP 005 **Rapid Drug Detection by Ultrasonic Nebulizer Coupled with Atmospheric-Pressure Chemical Ionization for Food-Product Analyses**; Linxia Song[1]; Yi You[2]; Theresa Evans-Nguyen[3]; *[1]University of Florida, Tampa, FL; [2]Federal Institute for Materials Research and Testing (BAM), Berlin, Germany; [3]University of South Florida, Tampa, FL*

WP 006 **A Novel Approach to Simultaneous Quantification of Tropane Alkaloids in Plant Tissue (Datura spp.) Using DART-HRMS and PLS Linear Regression**; Samira Beyramysoltan[1]; Rabi A. Musah[1]; *[1]Department of Chemistry, State University of New York at Albany, Albany, NY*

WP 007 **A Coated Blade Spray - Mass Spectrometry (CBS-MS) Method for Simultaneous Screening of 68 Drugs and Metabolites in Urine**; Shirin Hooshfar[1]; Simone Tchu[1]; German A. Gómez-Ríos[2, 3]; Daniel A. Rickert[3]; Janusz Pawliszyn[3]; Kara Lynch[1]; *[1]University of California, San Francisco (UCSF), San Francisco, CA; [2]Restek Corporation, Bellefonte, PA; [3]University of Waterloo, Waterloo, ON*

WP 008 **Real-Time Analysis of the Metabolic Profile of Microglia Using Liquid Microjunction Surface Sampling Coupled with High-Resolution Mass Spectrometry**; Taylor M. Domenick[1]; Vinata Vedam-Mai[1]; Timothy J. Garrett[1]; Richard A. Yost[1]; *[1]University of Florida, Gainesville, FL*

WP 009 **DART-MS: Enabling Safer Reaction Monitoring and Analysis Conditions with In Hood Vaporization**; Brittany Laramee[1]; Frederick Li[1]; Paul Liang[1]; Brian Musselman[1]; *[1]IonSense, Inc, Saugus, MA*

WP 010 **High Throughput 96-Pin Solid Phase Microextraction Array for Direct Analysis in Real Time**; Paul Liang[1]; Frederick Li[1]; Brittany Laramee[1]; Brian Musselman[1]; *[1]IonSense, Inc, Saugus, MA*

WP 011 **Can Reducing Sample Volume and Desorption Time Lead during Ambient Ionization lead to Improved Drug Detection from Biological Fluids**; Brian D. Musselman[1]; Paul Liang[2]; *[1]IonSense, Inc., Saugus, MA; [2]IonSense,Inc., Saugus, MA*

WP 012 **The Eight(y) Million Pound Question: Using DESI Ambient MS Imaging for the Forensic Analysis of Cheque Fraud**; Huiqin Zhong[1]; Zhengwei Jia[1]; Wei Rao[1]; *[1]Waters Technologies (Shanghai) Co., Ltd, Shanghai, China*

WP 013 **Rapid Screening of New Synthetic Drugs in Plasma Samples Using Paper Spray Mass Spectrometry with Integrated Solid-Phase Extraction Cartridge**; Greta J. Ren[1]; Brandon J. Bills[1]; Nicholas E. Manicke[1]; *[1]IUPUI Department of Chemistry & Chemical Biology, Indianapolis, IN*

WP 014 **Sub-Microliter Metabolomics via Triboelectric Nanogenerator-Induced Nanospray Mass Spectrometry**; Yafeng Li[1]; Marcos Bouza Areces[1]; Changsheng Wu[2]; Danning Huang[1]; Gilad Doron[3]; Johnna S Temenoff[3, 4]; Arlene A. Stecenko[5]; Zhong Lin Wang[2, 6]; Facundo M. Fernandez[1, 7]; *[1]School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA; [2]School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, Georgia; [3]W.H. Coulter Department of Biomedical Engineering, Georgia Institute of Technology and Emory University, 315 Ferst Drive, Atlanta, GA 30332,, Atlanta, Georgia; [4]Petit Institute for Bioengineering and Bioscience, Georgia Institute of Technology, Atlanta, Georgia; [5]Emory+Children's Center for Cystic Fibrosis and Airways Disease Research and Department of Pediatrics, Emory University School of Medicine and Children's Healthcare of Atlanta, Atlanta, Georgia; [6]Beijing Institute of Nanoenergy and Nanosystems, Chinese Academy of*

Sciences, Beijing, China; [7]Petit Institute of Bioengineering and Biosciences, Georgia Institute of Technology, Atlanta, Georgia

WP 015 **Ambient Mass Spectrometry Immunoassays Using Small-Molecule Signal Amplifiers for Zeptomole Protein Detection**; Shuting Xu[1]; Wen Ma[1]; Yu Bai[1]; Huwei Liu[1]; *[1]Peking University, Beijing, China*

WP 016 **Nitrogen and Ion Source Parameters: Considerations for Nitrogen Direct Analysis in Real Time**; Frederick Li[1]; Paul Liang[1]; Brittany Laramee[1]; Brian Musselman[1]; *[1]IonSense,Inc., Saugus, MA*

WP 017 **Molecular Level Identification of Soil Organic Matter from Polar Region by solid phase LDI-FTICR-MS**; Seulgidaun Lee[1]; Sunghwan Kim[1]; *[1]Kyungpook National University, Daegu, South Korea*

WP 018 **Lower Detection Limits for Paper Spray Mass Spectrometry Using on Paper Extraction**; Brandon Bills[1]; Nicholas E. Manicke[1]; *[1]IUPUI Department of Chemistry & Chemical Biology, Indianapolis, IN*

WP 019 **Rapid Identification of Wuyi Rock Tea Regions using the Direct Analysis in Real Time (DART) MS System with LiveID**; Yuhong Qin[1]; Wei Rao[1]; Huiqin Zhong[1]; Fang Shu[1]; Zhengwei Jia[1]; Defeng Huang[1]; Clara Chen[1]; Kate Yu[1]; *[1]Waters Technologies (Shanghai) Co, Ltd, Shanghai, China*

WP 020 **Acoustic Mist Ionisation (AMI) a Rapid Approach for the Development of Mass Spectrometry Libraries**; Michael McCullagh[1]; Sara Stead[1]; Gareth Rhys Jones[1]; Michelle Wood[1]; Severine Goscinny[2]; Nayan Mistry[1]; Kenneth Rosnack[3]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Sciensano, Brussels, Belgium; [3]Waters Corporation, Milford, MA*

WP 021 **A Validated Method for Quantification of Mescaline in Recreationally-abused EchinopsisCacti by Direct Analysis in Real Time Mass Spectrometry**; Cameron Longo[1]; Rabi A. Musah[1]; *[1]University at Albany - SUNY, Albany, NY*

WP 022 **Detection of Organometallic Compounds on a Waters QDa Mass Spectrometer Equipped with a Helium-Plasma-Ionization (HePI) Source**; Athula B. Attygalle[1]; Julius Pavlov[1]; David Douce[2]; Steve Bajic[3]; *[1]Stevens Institute of Technology, Hoboken, NJ; [2]Waters corporation, Wilmslow, United Kingdom; [3]Waters Corporation, Wilmslow, United Kingdom*

WP 023 **Rapid Quantitative Analysis of Six Anti-arrhythmic Drugs in Human Serum Using Direct Analysis in Real Time Mass Spectrometry**; Yuzhou Gui[1]; Xiaokun Duan[2]; Kerry Song[2]; Jiale Xu[2]; Charles C. Liu[2]; Hong Yan[3]; Youli Lu[1]; Gangyi Liu[1]; *[1]Central Laboratory, Shanghai Xuhui Central Hospital/Zhongshan - Xuhui Hospital, Fudan University /Shanghai Clinical Center, Chinese Academy of Sciences, Shanghai, China; [2]ASPEC Technologies Limited, Beijing, China; [3]Shanghai Institute of Medical Genetics, , Shanghai Children's Hospital, Shanghai Jiao Tong University School of Medicine, Shanghai, China*

WP 024 **Direct insertion probe and atmospheric pressure ionization coupled to high-resolution mass spectrometry for the description of lignocellulosic biomass**; Clément Castilla[1]; Christopher P. Rüger[1]; Hélène Lavanant[1]; Carlos Afonso[1]; *[1]Normandie Univ, INSA Rouen, UNIROUEN, CNRS, COBRA, Rouen, France, Rouen, France*

WP 025 **A Prototype Direct Sampling Inlet for the Rapid Analysis of Target Analytes in the Chemical Industry**; Rachel Sanig[1]; David Douce[1]; Jeff Goshawk[1]; Caitlyn Da Costa[1]; Gordon Jones[1]; Eleanor Riches[1]; *[1]Waters Corporation, Wilmslow, United Kingdom*

WP 026 **Ambient Ionisation Mass Spectrometry: A novel diagnostic tool for debugging electronic circuits**; Barry Smith[1]; Cedric Boisdon[1]; Simon Maher[1]; *[1]University of Liverpool, Liverpool, United Kingdom*

WP 027 **Wood Discrimination Analyses of Pterocarpus tinctorius and Endangered P. santalinus Using DART-FTICR-MS Coupled with Multivariate Statistics**; Maomao Zhang[1,2]; Yafang Yin[1,2]; Wen Zhou[3]; Jiang Zhou[3]; Xiaokun Duan[4]; Charles C. Liu[4]; *[1]Department of Wood Anatomy and Utilization, Research Institute of Wood Industry, Chinese Academy of Forestry, Beijing, China; [2]Wood Collections (WOODPEDIA), Chinese Academy of Forestry, Beijing, China; [3]Peking University, Beijing, China; [4]ASPEC Technologies, Beijing, China*

WP 028 **Direct Analysis in Real Time Mass Spectrometry and Multivariate Data Analysis for Profiling of Chinese Propolis**; Yilei Huang[1]; Zhongping Huang[1]; Charles C. Liu[2]; Kezhi Jiang[3]; Lili Wang[4,1]; Xiaokun Duan[2]; *[1]Zhejiang University of Technology, Hangzhou, China; [2]ASPEC Technologies, Beijing, China; [3]Hangzhou Normal University, Hangzhou, China*

WP 029 **Intact Metabolomics by PESI/MS/MS and its Application to Metabolic Profiling of Acetaminophen-Induced Acute Hepatic Injury Model Mice**; Tomomi Ohara[1]; Kenta Kondo[1]; Tasuku Murata[2]; Tetsuya Ishikawa[3]; Akira Ishii[1]; Hitoshi Tsuchihashi[1]; Koretsugu Ogata[2]; Yumi Hayashi[3,4]; Kei Zaitsu[1,4]; *[1]Department of Legal Medicine and Bioethics, Nagoya University Graduate School of Medicine, Nagoya, Japan; [2]Shimadzu Corporation, Kyoto, Japan; [3]Pathophysiological Laboratory Sciences, Department of Radiological and Medical Laboratory Sciences, Nagoya University Graduate School of Medicine, Nagoya, Japan; [4]In Vivo Real-Time Omics Laboratory, Institute for Advanced Research, Nagoya University, Nagoya, Japan*

WP 030 **Rapid Analysis of Drugs in Plasma Using Probe Electrospray Ionization Mass Spectrometry**; Hidekazu Saiki[1]; Tasuku Murata[1]; Koretsugu Ogata[1]; Takahiro Inoue[2]; Kenji Nakayama[3]; Koji Shimizu[2]; Osamu Ogawa[2]; *[1]Shimadzu corp., Kyoto, Japan; [2]Kyoto University, Kyoto, Japan; [3]Shimadzu Techno-Research, Inc., Kyoto, Japan*

WP 031 **Direct Analysis of Cell Wall Lipids from Mycobacteriumvia LESA-MS**; Rian L Griffiths[1]; Luke Alderwick[2]; *[1]University of Nottingham, Nottingham, United Kingdom; [2]University of Birmingham, Birmingham, United Kingdom*

ANTIBODIES & ANTIBODY DRUG CONJUGATES II
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WP 032 **MALDI-In-Source Decay FT-ICR MS for Top-Down and Middle-Down Characterization of Monoclonal antibodies**; Christoph J. Gstöttner[1]; Yuri E.M. van der Burgt[1]; David P. A Kilgour[2]; Yury Tsybin[3]; Manfred Wuhrer[1]; Simone Nicolardi[1]; *[1]Center for Proteomics and Metabolomics, LUMC, Leiden, Netherlands; [2]Department of Chemistry, Nottingham Trent University, Nottingham, United Kingdom; [3]Spectroswiss, Lausanne, Switzerland*

WP 033 **A Comparative Study of N-Glycosylation Assays for the Characterization of Fc and Fab N-Glycans on Monoclonal Antibodies**; John F. Kelly[1]; Tammy-Lynn Tremblay[1]; Denis Brochu[1]; Robotham Anna[1]; *[1]Human Health Therapeutics, National Research Council of Canada, Ottawa, ON*

WP 034 **MS-based Characterization of a Novel Antibody Against Marburg Virus Nucleoprotein**; yanchun Lin[1]; Britney Johnson[2]; Angela Zou[2]; Kathleen C.F. Sheehan[2]; Gaya Amarasinghe[2]; Daisy Leung[2]; Michael L. Gross[1]; *[1]Department of Chemistry, Washington University in St Louis, St Louis, MO; [2]Department of Pathology and Immunology, Washington University School of Medicine, St Louis, MO*

WP 035 **Rapid Conjugation, Proteolysis and Purification of Antibodies Using High Capacity CapturemTM Membranes**; Christian Hoppmann[1]; Mandy Li[1]; Michael Vierra[1]; Boris Levitan[1]; Gia Jokhadze[1]; Andrew Farmer[1]; *[1]Takara Bio USA, Mountain View, CA*

WP 036 **Quantitative MFLC-MS/MS Analysis of the Antibody Drug Conjugate SigmaMAb Extracted from Rat Plasma Using Thermo Scientific MSIA Microcolumns**; Chad Christianson[1]; Jennifer Zimmer[1]; Kwasi Antwi[2]; Chris Ross[2]; Shane R Needham[1]; *[1]Alturas Analytics, Moscow, ID; [2]Thermo Fisher Scientific, West Palm Beach, FL*

WP 037 **Top-down Proteogenomics Analysis of Serum Autoantibody Repertoire for the Discovery of Biomarker of Systemic Lupus Erythematosus**; Zhe Wang[1]; Xiaowen Liu[2]; Kenneth Smith[3]; Si Wu[1]; *[1]University of Oklahoma, Norman, OK; [2]Indiana University-Purdue University Indianapolis, Indianapolis, IN; [3]Oklahoma Medical Research Foundation, Oklahoma City, OK*

WP 038 **High Sensitivity Native Analysis of Monoclonal antibodies by Electrokinetically Pumped Sheath-Flow Capillary Zone Electrophoresis-Mass Spectrometry on a Q-TOF Mass Spectrometer**; Xiaojing Shen[1]; Zhichang Yang[1]; David Wong[2]; Qiangwei Xia[3]; Liangliang Sun[1]; *[1]Michigan State University, East Lansing, MI; [2]Agilent Technologies, Santa Clara, CA; [3]CMP Scientific Corp, New York, NY*

WP 039 **Characterization of Monoclonal Antibody Biosimilar through C-terminal and Disulfide Bond PeptidesSequencing Analysis on Q-TOF Mass Spectrometer**; Udi Jumhawan[1]; Zhaoqi Zhan[1]; *[1]Shimadzu Asia Pacific, Singapore, Singapore*

WP 040 **Application of a Label-Free and Domain-Specific Free Thiol Method In Monoclonal Antibody Characterization**; Yi Pu[1]; Yunqiu Chen[1]; Tai Nguyen[1]; Chong-Feng Xu[1]; Li Zang[1]; Zoran Sosic[1]; Tyler Carlage[1]; *[1]Biogen, Cambridge, MA*

WP 041 **Enabling Single-cell Clone Selection for Knob-in-Hole Bispecific Antibodies via Automated Affinity Capture Coupled to High-throughput RapidFire Mass Spectrometry**; William Sawyer[1]; Neha Srikumar[2]; Joseph Carver[2]; Phillip Y. Chu[2]; Amy Shen[2]; Ankai Xu[2]; Ambrose Williams[2]; Cong Wu[2]; Yichin Liu[2]; John C. Tran[2]; *[1]Genentech, South San Francisco, CA; [2]Genentech, Inc., South San Francisco, CA*

WP 042 **Towards Better Characterizing Drug-Antibody Ratios in Antibody-Drug Conjugates with Ion Mobility Separations in Structures for Lossless Ion Manipulations**; Gabe Nagy[1]; Isaac K. Attah[1]; Yue-Mei Zhang[2]; James Lanter[2]; Jared B. Shaw[1]; Sandilya V. B. Garimella[1]; Harsha P. Gunawardena[2]; Richard D. Smith[1]; Yehia M. Ibrahim[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Janssen Research and Development, Spring House, PA*

WP 043 **Regulated LCMS bioanalysis of Monoclonal Antibodies in Human Serum for Inflammatory Immune Disease Management Using Novel Fab-Selective nSMOL Chemistry**; Noriko Iwamoto[1]; Atsushi Yonezawa[2,3]; Kazuo Matsubara[3]; Takashi Shimada[1,4]; *[1]Shimadzu Scientific Instruments, Bothell, WA; [2]Kyoto University, Kyoto, Japan; [3]Kyoto University Hospital, Kyoto, Japan; [4]Shimadzu Corporation, Kyoto, Japan*

WP 044 **A Proteomic Approach to Single Chain Camelid Antibody Discovery**; Anand Patel[1]; Natalie Castellana[1]; Thiago Lima[1]; Stefano Bonissone[1]; *[1]Digital Proteomics, LLC., San Diego, CA*

WP 045 **Affinity Based LC-MS Method for Improved Determination of HCP-ELISA Reagent Coverage**; Christina Seisenberger[1]; Stefanie Wohlrab[1]; *[1]Roche Diagnostics GmbH, Penzberg, Germany*

WP 046 **A Large Scale Comparison of MS-based Antibody De Novo Protein Sequencing and Targeted DNA Sequencing**; Zac McDonald[1]; Signy Chow[2,3]; Kathleen Gorospe[1]; Xin Xu[1]; Paul Taylor[1]; Qixin Liu[1]; Trevor J Pugh[2]; Suzanne Trudel[2]; Bin Ma[1]; *[1]Rapid Novor Inc., Kitchener, ON; [2]University Health Network/Princess Margaret Hospital, Toronto, ON; [3]Sunnybrook Health Sciences Centre, Toronto, ON; [4]University of Waterloo, Waterloo, ON*

WP 047 **Exploring the Effects of Media on Glycosylation of Biotherapeutics with Reduced Mass and Multi-Attribute Method (MAM) Analysis**; Yuko Ogata[1]; Nancy S Nightlinger[1]; Richard S Rogers[1]; *[1]Just Biotherapeutics, Seattle, WA*

WP 048 **Monitoring of DAR/ADC attributes for Trastuzumab Emtansine**; Sibylle Heidelberger[1]; Ferran Sanchez[2]; *[1]AB Sciex UK Ltd, Warrington, United Kingdom; [2]SCIEX, Madrid, Spain*

WP 049 **Rapid and Automated LCMS Characterization of Antibody and Protein Drug Conjugates**; Mark E. Hail[1]; Robert Schuster[1]; Kevin McCarl[1]; *[1]Novatia LLC, Newtown, PA*

WP 050 **Interactions of Hepatitis B Virus Capsids with Importin β and Anti-viral Drugs Monitored by Charge Detection Mass Spectrometry**; Christine Kim[1]; Nicholas A. Lyktey[1]; Adam Zlotnick[1]; Martin F. Jarrold[1]; *[1]Indiana University, Bloomington, IN*

WP 051 **In-Depth Characterization of *in vivo* Biotransformations for Trastuzumab Emtansine by Orbitrap MS**; Jintang He[1]; Shang-Fan Yu[1]; Sharon Yee[1]; Surinder Kaur[1]; Keyang Xu[1]; *[1]Genentech Inc., South San Francisco, CA*

WP 052 **Characterization of N-Glycan Species of VEGF Decoy Receptor Fusion Protein by Novel HILIC-LC Separation with High Sensitive Mass Spectrometric Characterization**; Mihir Mahendra Thakar[1]; Faraz Rasid[2]; Dipankar Malakar[2]; Bobby Virasingh[1]; Manoj Pillai[2]; *[1]Phenomenex India Pvt Ltd, Hyderabad, India; [2]SCIEX INDIA, GURUGRAM, India*

WP 053 **Affinity Purification of IdeZ Digest for Glycosylation Profile of Immunoglobulins Using a Linear Benchtop MALDI-TOFMS**; Yuzo Yamazaki[1]; Shuichi Nakaya[1]; *[1]Shimadzu Corporation, Kyoto, Japan*

WP 054 **Investigation of Ocular Tissue Disposition of Antibody-Drug Conjugates Using Novel LC-MS-Based Strategies**; Xiaoyu Zhu[1]; Ming Zhang[2]; Jie Pu[1]; Shihan Huo[1]; Chao Xue[1]; Jun Qu[1,2]; *[1]University at Buffalo, Buffalo, NY; [2]New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, New York*

WP 055 **Strategies for Sample Handling and Characterization of Antibody-Drug Conjugates by Quadrupole Mass Spectrometry**; Malin Källsten[1,2]; Matthijs Pijnappel[2]; Rafael Hartmann[1,2]; Fredrik Lehmann[3]; Lucia Kovac[2]; Sara Bergström Lind[1]; Jonas Bergquist[1]; *[1]Uppsala University, Uppsala, Sweden; [2]Recipharm OT Chemistry AB, Uppsala, Sweden; [3]Oncopeptides AB, Stockholm, Sweden*

WP 056 **Optimization of a LC/MS Method for Disulfide Characterization and Free Cystine Quantification in Protein Therapeutics**; Song Nie[1]; Xin Chen[1]; Jun Lun[1]; *[1]Catalent Pharma Solutions, Madison, WI*

WP 057 **A New Preparation Method Enabling Targeted Quantification of Biotherapeutics, Biomarker/Target Levels in FFPE Tissues with High Protein Recovery and Reproducibility**; Chao Xue[1]; Jie Pu[1]; Shihan Huo[1]; Xiaoyu Zhu[1]; Ming Zhang[2]; Jun Qu[1,2]; *[1]University at Buffalo, Buffalo, NY; [2]New York State Center of Excellence in Bioinformatics & Life Sciences, Buffalo, New York*

WP 058 **Cleavage of Intact Monoclonal Antibodies by Cathepsin L and D Studied by Native Mass Spectrometry**; Wilfred Tang[1]; Marshall Bern[1]; Andrew C Nichols[1]; Jing Zhu[2]; Tomislav Caval[2]; Albert J.R. Heck[2]; *[1]Protein Metrics Inc., Cupertino, CA; [2]Utrecht University, Utrecht, Netherlands*

WP 059 **High Resolution MS-based Structural Characterization Plays a Key Role in ADC Process Development**; Zhiqi Hao[1]; Diana Y. Liu[1]; Qiuting Hong[2,3]; Michael Kim[1]; William Haskins[1,4]; Tomasz Baginski[1]; Yan Chen[1]; *[1]Genentech,*

South San Francisco, CA; [2]Eurofins Lancaster Laboratories, Inc., Lancaster, PA; [3]Allakos Inc., Redwood City, CA; [4]Gryphon Bio Inc, South San Francisco, CA

WP 060 **Development of a Fully Automated Peptide Mapping Procedure**; Chen Qian[1]; Rob Brian Jimenez[1]; Ben Niu[1]; Methal Albarghouthi[1]; *[1]MedImmune, Gaithersburg, MD*

WP 061 **Assessment of Anti-drug Antibodies in Cynomolgus Monkey Dosed with an Antibody Drug Conjugate Using Immunocapture-LC/MS**; Luying Chen[1, 2]; Linlin Dong[1]; Nicole Bebrin[1]; Hiroshi Sugimoto[1]; Martin Paton[1]; Dong Wei[1]; Mark Qian[1]; *[1]Takeda Pharmaceuticals International, Inc., Cambridge, MA; [2]Linus Pauling Institute, College of Pharmacy, Oregon State University, Corvallis, OR*

WP 062 **Antibody Subunit LC-MS Analysis from Pre-Clinical Studies for Biotransformation & Catabolism Determination**; John Kellie; *GSK, King Of Prussia, PA*

WP 063 **Using Low-Resolution MS for Protein Therapeutic Process Monitoring during Development after One-Time Characterization with High-Resolution MS**; Chien-Hsun Chen[1]; Eike Zimmermann[1]; Kenji Furuya[1]; Scott Corley[1]; *[1]Boehringer Ingelheim, Fremont, CA*

WP 064 **A novel Immunocapture Middle-Up LC-MS Method to Evaluate the *in vivo* Stability of Fc Conjugated Antibody Drug Conjugates (ADCs)**; Srikanth Kotapati[1]; David Passmore[1]; Qiang Cong[1]; Yam B Poudel[1]; Mei-Chen Sung[1]; Mary Huber[1]; Patrick Holder[1]; Sayumi Yamazoe[1]; Sanjeev Gangwar[1]; Chetana Rao[1]; Vangipuram S. Rangan[1]; Chin Pan[1]; Pina M. Cardarelli[1]; Shrikant Deshpande[1]; Pavel Strop[1]; Gavin Dollinger[1]; Arvind Rajpal[1]; *[1]Bristol-Myers Squibb, Redwood City, CA*

BIOMARKERS: DISCOVERY II
065-095

WP 065 **A Flexible Analytical Platform for the Discovery of Biomarkers of Disease**; Laura McGregor[1]; Pete Grosshans[1]; Anthony Buchanan[1]; Bob Green[1]; Nick Bukowski[1]; *[1]SepSolve Analytical, Peterborough, United Kingdom*

WP 066 **The Discovery of Potential Cancer Biomarkers in Human Plasma Using GC- and GCxGC-TOFMS**; David E Alonso[1]; Habtom Ressom[2]; Cristina Di Poto[2]; Joseph E Binkley[3]; *[1]Leco Corporation, St. Joseph, MI; [2]Georgetown University Medical Center, Washington, DC; [3]LECO Corporation, St Joseph, MI*

WP 067 **AlbuVoid™ Enrichment & Antibody Depletion - Solving the Challenges of Serum Proteomics**; Matt Kuruc[1]; Swapan Roy[1]; Haiyan Zheng[2, 3]; Amenah Soherwardy[2, 3]; *[1]Biotech Support Group LLC, Monmouth Junction, NJ; [2]Rutgers University, New Brunswick, NJ; [3]Rutgers Proteomics Center, Piscataway, NJ*

WP 068 **Applications of SurfaceGenie: A Web-Based Tool for Mining Experimental Data for Informative Surface Proteins**; Matthew Waas[1]; Shana T. Snarrenberg[1]; Jack Littrell[1]; Rebekah L. Gundry[1]; *[1]Medical College of Wisconsin, Milwaukee, WI*

WP 069 **Plasma Proteins as New Biomarkers of Irradiation in Humans**; Ales Tichy[1]; Gabriela Kultova[1, 2]; Helena Rehulkova[1, 2]; Pavel Rehulka[1]; Alena Myslivcova-Fucikova[1, 2]; *[1]University of Defence, Hradec Kralove, Czech Republic; [2]University of Hradec Králové, Czech Republic, Hradec Králové, Czech Republic*

WP 070 **Global Plasma Proteome Quantification Using Internal Standard Triggered Targeted Analyses**; Sebastien Gallien[1, 2]; Jing Wang[1]; Aaron S. Gajadhar[3]; Bhavin Patel[4]; Markus Kellmann[5]; Tabiwang N. Arrey[5]; Alexander Harder[5]; Romain Huguet[3]; Graeme McAlister[3]; Derek Bailey[3]; Shannon Eliuk[3]; Yue Xuan[5]; Andreas Huhmer[3]; Emily I. Chen[1]; *[1]Thermo Fisher Scientific, Precision Medicine Science Center, Cambridge, MA; [2]Thermo Fisher Scientific, Paris, France; [3]Thermo Fisher Scientific, San Jose, CA; [4]Thermo Fisher Scientific, Rockford, IL; [5]Thermo Fisher Scientific, Bremen, Germany*

WP 071 **Modification of Lipid Expression in human Clear Cell Renal Cell Carcinoma**; Lucia Martin-Saiz[1]; Olatz Fresnedo[2]; Jone Garate[1]; Roberto Fernandez[1]; Peio Errarte[3]; Maider Beitia[3]; Gorka Larrinaga[3]; Jon Danel Solano-Iturri[4]; Beatriz Abad[5]; Jose Andrés Fernández[1]; Begoña Ochoa[2]; *[1]Dep. of Physical Chemistry, Fac. of Science and Technology, University of the Basque Country (UPV/EHU), Leioa, Spain; [2]Department of Physiology, Fac. of Medicine and Nursing, University of the Basque Country(UPV/EHU), Leioa, Spain; [3]Department of Nursing, Fac. of Medicine and Nursing, University of the Basque Country (UPV/EHU),, Leioa, Spain; [4]Department of Pathology, Cruces University Hospital, Barakaldo, Spain; [5]Liquid Chromatography and lipidomics platform, SGIKER, University of the Basque Country (UPV/EHU), Leioa, Spain*

WP 072 **Amniotic Fluid Proteome of Neonates with Congenital Diaphragmatic Hernia**; Sumit Bhutada[1]; Karin Tran-Lundmark[2]; Carmen Mesas-Burgos[2]; Peter Conner[2]; Bjorn Frenckner[2]; Suneel Apte[1]; *[1]Cleveland Clinic, Cleveland, OH; [2]Karolinska Institutet, Stockholm, Sweden*

WP 073 **Characterizing Glycans and Glycan Isomers Associated with Breast Cancer Tissue Phenotypes**; Sakshi Gautam[1]; Wenjing Peng[1]; Xue Dong[1]; Jingfu Zhao[1]; Yifan Huang[1]; Aiying Yu[1]; jieqiang Zhong[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

WP 074 **Proteomic Profiling and Immunoassay-based Validation of Biomarkers in Human Plasma from Alzheimer's Patients**; Mei Chen[1]; Abby S. Gelb[1]; Weiming Xia[1, 2]; *[1]Geriatric Research Education and Clinical Center (GRECC), ENR Memorial Veterans Hospital, Bedford, MA; [2]Boston University School of Medicine, Boston, MA*

WP 075 **LC-MS/MS Proteomic: Identification of Candidate Biomarkers of Breast Cancer Subtypes**; Jingfu Zhao[1]; Wenjing Peng[1]; Aiying Yu[1]; Yifan Huang[1]; Xue Dong[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

WP 076 **Proteomic Profiling of Ovarian Cancer Extracellular Vesicles for Biomarker Discovery**; Dylan Z Dieters-Castator[1, 2]; Jiahui Liu[1]; Gilles Lajoie[2]; Lynne-Marie Postovit[1, 2]; *[1]University of Alberta, Edmonton, AB; [2]Western University, London, ON*

WP 077 **Multiplexed, Quantitative Proteomic Comparison of a Novel Nrf2 Pathway – Targeting Therapeutic Compound in Two Separate, but Complementary, Matrices**; Damon Young[1]; Amanda L. Edwards[1]; Sharon O'Neill[1]; Ashley Nelson[1]; Ankur Thomas[1]; Brian Wipke[1]; Michael Rooney[1]; Omar Mabrouk[1]; Danielle Graham[1]; *[1]Biogen, Cambridge, MA*

WP 078 **Identifying Novel Upstream Kinases of the Microtubule-Associated Protein Tau Using Fluorescence Complementation Mass Spectrometry (FCMS) in an Alzheimer's-like cell model**; Der-Shyang Kao[1]; Yanyan Du[2]; W. Andy Tao[2]; *[1]Purdue University, West lafayette, Indiana; [2]Purdue University, West Lafayette, Indiana*

WP 079 **Secretotranscriptomic Identification and Validation of New Prognostic Liquid Biopsy Biomarkers**; J. Astor Ankney[1]; John A. Wrobel[1]; Ling Xie[1]; Xian Chen[1, 2]; *[1]Department of Biochemistry and Biophysics, University of North Carolina, Chapel Hill, NC; [2]Lineberger Comprehensive Cancer Center, University of North Carolina at Chapel Hill, Chapel Hill, NC*

WP 080 **Region-Specific N-Glycome Mapping of the Human Brain in Alzheimer's Patients by nanoLC chip-Q-TOF MS Analysis**; Jennyfer Tena[1]; Mariana Barboza[1]; Maurice Wong[1]; Carlito B Lebrilla[1]; *[1]University of California, Davis, Davis, CA*

WP 081 **The Urinary Metabolome and Lipidome of Prostate Cancer**; Iqbal Mahmud[1]; Timothy J Garrett[1]; *[1]University of Florida Department of Pathology, Immunology, and Laboratory Medicine, Gainesville, FL*

WP 082 **Proteomic Discovery of Potential Biomarkers in Zika Virus Infected Monkeys;** Bao Q. Tran[1]; Gabrielle Rizzo[2]; Michael Ward[3]; Lisa Cazares[3]; Trevor Glaros[4]; *[1]20th CBRNE Command, APG, MD; [2]Excet, Inc., Springfield, VA; [3]United States Army Medical Research Institute of Infectious Diseases, Fort Detrick, MD; [4]ECBC, Aberdeen Proving Ground, Maryland*

WP 083 **Serum Proteomic Profiling for Biomarker Discovery in Ischemic Stroke;** Miji Shin[1]; Jiyeong Lee[2]; Arum Park[2]; Sora Mun[1]; You-rim Lee[1]; Ae Eun Seok[2]; Hyo-jin Kim[1]; Yoo-jin Lee[1]; Hee-gyoo Kang[1,2]; *[1]Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Daejeon, South Korea; [2]Department of Biomedical Laboratory Science, College of Health Sciences, Eulji University, Seongnam-si, South Korea*

WP 084 **Phosphatidylcholines as a Biomarker Potential Candidate of Multiple Sclerosis;** Fernando Brunale Leite[1]; Danielle Zildeana Furtado[1]; Cleber Nunes Barreto[1]; Erica Souza Silva[1]; Nilson Antonio Assuncao[1]; *[1]Unifesp, São Paulo, Brazil*

WP 085 **Proteome and Phosphoproteome Biomarker Discovery Strategies for Biopsy-Free Bladder Cancer Diagnosis Based on Urinary Extracellular Vesicles;** Xiaofeng Wu[1]; Sebastian Paez[1]; Hristos Kaimakliotis[2]; Anton B. Iliuk[3]; Weiguo Andy Tao[1]; *[1]Purdue University, West Lafayette, IN; [2]Indiana University School of Medicine, Indianapolis, Indiana; [3]Tymora Analytical Operations, West Lafayette, IN*

WP 086 **Aging Markers and Ageotypes Revealed by Deep Longitudinal Profiling;** Sara Ahadi[1]; Wenyu Zhou[1]; Reza Sailani[1]; Kevin Contrepois[1]; Michael Snyder[1]; *[1]Stanford University School of Medicine, Stanford, CA, 94305*

WP 087 **Deciphering Racial Disparities in Breast Cancer by Novel Extracellular Matrix Proteomic Approaches on Formalin-Fixed, Paraffin-Embedded Clinical Specimens;** Peggi M. Angel[1]; Baylye Boxall[1]; Jennifer R. Bethard[1]; Lauren E. Ball[1]; Jeffrey R. Marks[2]; Richard R. Drake[1]; *[1]Medical University of South Carolina, Charleston, SC; [2]Duke University School of Medicine, Durham, NC*

WP 088 **Stability-Based Protein Fractionation of Plasma Reveals Insights into Familial Amyloid Polyneuropathy Treatment with Tafamidis;** Jolene K Diedrich[1]; Chung-Yon Lin[1]; Jeffery W Kelly[1]; John R. Yates, III[1]; *[1]The Scripps Research Institute, La Jolla, CA*

WP 089 **Serum Proteomic Profiling for Biomarker Discovery in Rheumatoid Arthritis;** Sora Mun[1]; Jiyeong Lee[2]; Arum Park[2]; Ae Eun Seok[2]; Hyo-jin Kim[1]; Yoo-jin Lee[1]; Hee-gyoo Kang[1,2]; You-rim Lee[1]; *[1]Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Daejeon, South Korea; [2]Department of Biomedical Laboratory Science, College of Health Sciences, Eulji University, Seongnam-si, South Korea*

WP 090 **Development of a Bioanalytical Method for the Measurement of Symmetric-Dimethylarginine (SDMA) in Formalin-Fixed Paraffin-Embedded (FFPE) and Frozen Samples by LC/MS/MS;** Max Lein[1]; David Pirman[1]; Gina Lein[2]; Katherine Sellers[1]; Everton Mandley[1]; Taryn Sleger[1]; Katya Marjon[1]; Guowen Liu[1]; Yue Chen[1]; *[1]Agios Pharmaceuticals, Cambridge, MA; [2]Sigilon Therapeutics, Cambridge, MA*

WP 091 **UTIDx: 60 Second Assay for Detecting Urinary Tract Infections;** Dominique G Bihan[1]; Spencer D Wildman[1]; Daniel B Gregson[2]; Thomas Rydzak[1]; Ryan A Groves[1]; Carly Y Chan[1]; Deirdre L Church[2]; Ian A Lewis[1]; *[1]University of Calgary, Calgary, AB; [2]Calgary Laboratory Services, Alberta Health Services, Calgary, AB*

WP 092 **A Tunable Approach for Median-Polish of Ratio (TAMPOR) across Batches of Proteomics Datasets Deals a Blow to Stubborn Technical Variance;** Eric B Dammer[1,2,3]; Tyler W.A. Bradshaw[4]; Lenora A Higginbotham[3,5]; Lingyan Ping[3,5,6]; Duc M Duong[2,3,5]; James J. Lah[3,5]; Allan I. Levey[3,5]; Scott H Soderling[4]; Nicholas T. Seyfried[2,3,5]; *[1]Emory University, Atlanta, GA; [2]Emory Integrated Proteomics Core, Emory University, Atlanta, Georgia; [3]Emory School of Medicine, Atlanta, GA; [4]Duke University School of Medicine, Durham, NC; [5]Emory University - Center of Neurodegenerative Diseases, Atlanta, GA; [6]Emory University-Biochemistry, Atlanta, GA*

WP 093 **Metabolomic Approach for the Discovery of Internal Standard Substances of Bloodstain;** Hee-gyoo Kang[1,2]; You-rim Lee[1]; Jiyeong Lee[1]; Ae Eun Seok[1]; Arum Park[1]; Sora Mun[1]; Hyojin Kim[1]; Yoo Jin Lee[1]; *[1]Department of Senior Healthcare, BK21 Plus Program, Graduate School, Eulji University, Daejeon, South Korea; [2]Department of Biomedical Laboratory Science, College of Health Sciences, Eulji University, Seongnam-si, South Korea*

WP 094 **Lipid Signature to Distinguish between Patient with type II Diabetes and Type II Diabetes with Cardiovascular Disease;** yashwant kumar; *Translational health science and technology institute, Faridabad, India*

WP 095 **Proteomic Analysis of NMuMG Cells Undergoing Epithelial Mesenchymal Transition;** Santanu Palchaudhri[1]; Faraz Rashid[2]; Dipankar Malakar[2]; Manoj G Pillai[2]; *[1]Amity University, Kolkata, India; [2]SCIEX, Gurgaon, India*

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WP 096 **A Sensitive and RobustUPLC-MS/MS Methodfor Quantitation of Estrogens and Progestogensin HumanSerum;** Junmei Zhang[1]; Chenxiao Tang[1]; Patrick J. Oberly[1]; Margaret B. Minnigh[1]; Sharon L. Achilles[1,2]; Samuel M. Poloyac[1]; *[1]University of Pittsburgh, Pittsburgh, PA; [2]Magee-Womens Research Institute, Pittsburgh, PA*

WP 097 **Identification of Candidate Biomarkers for Head and Neck Cancer Using LC-SRM and Longitudinal Samples from the DOD Serum Repository;** Ju Yeon Lee[1]; Tujin Shi[1]; Vladislav Petyuk[1]; Athena Schepmoes[1]; Thomas Fillmore[1]; Wayne Cardoni[2]; George Coppit[2]; Joseph Goodman[2]; Shiv Srivastava[3]; Craig Shriver[2]; Tao Liu[1]; Karin Rodland[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Walter Reed National Military Medical Center, Bethesda, MD; [3]Center for Prostate Disease Research, Bethesda, MD*

WP 098 **Assessment of Food Impact on Serum Bile Acid Changes in a clinical methodology study by LC-MS/MS Analysis;** Lina Luo[1]; John Pettersen[2]; Michael Aleo[1]; Christopher Holliman[1]; Ragu Ramanathan[1]; *[1]Pfizer WRD, Groton, CT; [2]University of Connecticut, Storrs, CT*

WP 099 **TNF-α Regulated Metabolic Reprograming in Breast Cancer Using High-Resolution Proteomics;** Ha Yun Lee[1,2]; Eugene C. Yi[1,2]; Kritarth Singh[3]; Rajesh Singh[3]; Hanbyeol Kim[4]; *[1]Seoul national university, Seoul, South Korea; [2]Department of Molecular Medicine and Biopharmaceutical Sciences, Graduate School of Convergence Science and Technology, Seoul National University, Seoul, South Korea; [3]Department of Bio-Chemistry, The M.S. University of Baroda, Vadodara, India; [4]Department of Integrated OMICS for Biomedical Science, Graduate School, Yonsei University, seoul, South Korea*

WP 100 **Identification *Clostridum chauvoei* by MALDI-TOF MS from Paraffin Embedded Sections of Lower Extremity Infections, in Three Diabetes Patients after Amputations;** Barbara Dominiak[1]; Maria Anita Mendes[2,3,4,5]; *[1]Temple University, Philadelphia, PA; [2]Dampster Mass Spectrometry Lab, Sao Paulo-SP,, Brazil; [3]William Oxberry, Brooklyn, New York, SUNY Downstate Medical Center; [4]Patrick Chen, Brooklyn, SUNY Downstate Medical Center, New York; [5]Ernique ER Sanches, Dampster Mass Spectrometry Lab., Brazil*

WP 101 **Pre-Analytical Variation and Sample Quality Control of Human Blood for Metabolomics**; Xinyu Liu; *Dalian Institute OF Chemical Physics, Chinese Academy of Sciences, Dalian, China*

WP 102 **Surface Modification of Gold Nanoparticles and their Applications as Mass Tags for Protein Marker Detection in Laser Ionization Mass Spectrometry**; Siu Chung Toby Tam[1]; Yu-Hong Cheng[1]; Kwan-Ming Ng[1]; *[1]The University of Hong Kong, Hong Kong, Hong Kong*

WP 103 **Investigating Phytophthora methylation using Trapped Ion Mobility Spectrometry Mass Spectrometry**; Han Chen[1]; Qing Zhang[2]; Heiner Koch[3]; Lucy Woods[4]; Hongyu Ma[1]; *[1]Nanjing Agricultural University, Nanjing, China; [2]Bruker (Beijing) Scientific Technology Co., Ltd, Beijing, China; [3]Bruker Daltonik GmbH, Bremen, Germany; [4]Bruker Daltonics, 28359 Bremen, Germany*

WP 104 **Improvement of Phospho-monoester Lipids LC-MS Detection by Selective Capture using Molecularly Designed Materials**; Giuliana Grasso[1]; Carlo Crescenzi[1]; Börje Sellergren[2]; *[1]University of Salerno, Fisciano, Italy; [2]Biofilm Research Center for Biointerfaces, Malmö University, Malmö, Sweden, SE, Sweden*

WP 105 **Proteomic Analysis of Cerebrospinal Fluid in Alzheimer's disease**; Justin McKetney[1]; Daniel Panyard[1]; Sterling C Johnson[1]; Cynthia Carlsson[1]; Corinne D Engelman[1]; Joshua J Coon[1]; *[1]University of Wisconsin-Madison, Madison, WI*

WP 106 **Utilizing Blood Cards for Quantitative Assessment of Glutathione as an Important Biomarker Test for Autism Spectrum Disorder and Neurodegenerative Diseases**; Ashley Trouten[1]; H. m. Skip Kingston[1]; *[1]Duquesne University, Pittsburgh, PA*

WP 107 **Development of a Quantification Method for Intact Phosphorylated Alpha-Synuclein in Mouse Brain**; Jens Fogh[1]; François Fenaille[2]; Line Roerbaek Olsen[1]; Anne-Marie Jacobsen[1]; François Becher[2]; *[1]H. Lundbeck A/S, Valby, Denmark; [2]CEA Saclay, Service de Pharmacologie et Immunoanalyse (SPI) - Laboratoire d'Etude du Métabolisme des Médicaments, Gif-Sur-Yvette, France*

WP 108 **Rapid and Sensitive Derivatization Coupled with Ultra-High Performance Liquid Chromatography-Tandem Mass Spectrometry for Determination of α-Hydroxyglutaric Acid and α-Ketoglutaric Acid**; Hongmei Wang[1]; Shuai Li[1]; Sitan Xie[1]; Wuyun Gong[1]; Xiaotong Li[1]; Lili Xing[1]; Xin Zhang[1]; Yi Tao[1]; *[1]WuXi AppTec, Shanghai, China*

WP 109 **Targeted Mass Spectrometry Analysis of Gelsolin Isoforms in Duchenne Muscular Dystrophy**; michael Ogundele[1]; Emily Canessa[1]; Alison M Samsel[1]; Mansi V Goswami[1]; Tchilabalo D Alayi[1]; Yetrib Hathout[1]; *[1]University of Binghamton, Binghamton, NY*

WP 110 **Practical Procedure for Selecting an Appropriate Surrogate Matrix for Endogenous Peptide/ Protein Quantitation in Biomatrix via LC-MS/MS**; Moucun Yuan[1]; Jinlin Shen[1]; Omnia Ismaiel[1]; Eric Ma[1]; Michael Waldron[1]; William R. Mylott Jr.[1]; *[1]PPD, Richmond, VA*

WP 111 **Development of a CLIA-ready Protein Biomarker Assay Platform for Lung Cancer using LC-MRM Quantification**; Sandip Chavan[1]; Kiah Bowers[2]; Lancia Darville[2]; Bin Fang[2]; Sam Massoni[3]; Theresa Boyle[2]; Eric Haura[2]; John M. Koomen[2]; *[1]Moffitt Cancer Center, Tampa, FL; [2]Moffitt Cancer Center & Research Institute, Tampa, FL; [3]New England Peptide, Inc., MA, Gardner, Massachusetts*

WP 112 **Investigation of Plasma N-glycans Alteration in Dementia with Lewy Bodies**; Lang Ding[1]; Qi Zhang[2]; He Zhu[1]; Cheng Ma[1]; Lih-Shen Chin[2]; Lian Li[2]; Peng George Wang[1]; *[1]Georgia State University, Atlanta, GA; [2]Emory University, Atlanta, GA*

WP 113 **Between Scylla and Charybdis, A Journey to Find Optimal, Facile, Isotopic Standards for Plasma Biomarker Detection with MRM**; Mario M Alba[1]; Kym F Faull[2]; Kian Kani[1]; Alexander J Yoon[2]; Katrin Tiemann[1]; Carolina Garri[1]; Jack A Cipolla[2]; Jonathan E Katz[1]; *[1]Lawrence J. Ellison Institute for Transformative Medicine of USC, Los Angeles, California; [2]Jane and Terry Semel Institute for Neuroscience and Human Behavior and Department of Psychiatry and Biobehavioral Sciences at UCLA, Los Angeles, California*

WP 114 **Simultaneous Quantification of Nine Polyunsaturated Fatty Acids (PUFAs) in Rat Plasma by Reverse Phase LC-MS/MS**; Roger Pham[1]; Michelle Chen[2]; Josh Dekeyser[3]; Christopher A. James[2]; Omar S. Bamaby[2]; *[1]Amgen, Inc., Thousand Oaks, CA; [2]Amgen, Inc., Thousand Oaks, CA; [3]Amgen Inc., Boston, MA*

WP 115 **Redox Mass Tag for Absolute Quantitation in Mass Spectrometry**; Anyin Li[1]; Ran Qiu[1]; Xing Xu[2]; *[1]University of New Hampshire, Durham, NH; [2]University of New Hampshire, DURHAM, NH*

WP 116 **Development and Validation of an MS/MS Assay for Quantitation of Salivary Free Amino Acids in Volunteers Following Different Diet Regime**; Andrew Pinkham[1]; Hongqin Jiao[1,2]; Yanira E. Linberg[1]; Aaron Stairs[1]; Ewa Sokol[1]; *[1]Charles River Laboratories, Worcester, MA; [2]Charles River Laboratories, Shrewsbury, MA*

WP 117 **Protein Signatures of Seminal Plasma from Bulls with Contrasting Frozen-Thawed Sperm Viability**; Arlindo A. Moura[1,2]; Fabio F. Gomes[1]; Robin Park[1]; Carolina F. Costa[1]; Abdullah Kaya[3]; Erdogan Memili[4]; John R. Yates, III[1]; *[1]The Scripps Research Institute, La Jolla, CA; [2]Universidade Federal do Ceara, Fortaleza, Brazil; [3]Selcuk University, Selçuklu, Turkey; [4]Mississippi State University, Starkville, Mississippi*

WP 118 **Accelerated Workflow for Targeted SRM Assay Development from DIA Chromatogram Library: Targeted Assay for Parkinson's Disease Markers in Cerebrospinal fluid**; Eric L Huang[1]; Deanna Plubell[1]; Sandi Spencer[2]; Thomas Montine[3]; Michael J MacCoss[1]; *[1]University of Washington, Genome Sciences, Seattle, WA; [2]BC Cancer Research Agency, Vancouver, BC; [3]Department of Pathology, Stanford University, Stanford, CA*

WP 119 **Proteomics Analysis of Brain Meningiomas in Pursuit of Novel Biomarkers of the Aggressive Behavior**; Garni Barkhoudarian[1]; Julian Whitelegge[2]; Daniel Kelly[1]; Margaret Simonian[3]; *[1]John Wayne Cancer Institute, Providence St John's Health Center, Los Angeles, CA; [2]University of California LA, Los Angeles, CA; [3]University of California Los Angeles, Los Angeles, CA*

WP 120 **Post-Translationally Modified Proteins in Plasma Extracellular Vesicles as Candidate Markers for Breast Cancer Subtypes**; Hillary Andaluz Aguilar[1]; I-Hsuan Chen[1]; J. Sebastian Paez[1]; Anton B. Iliuk[2]; Sonia Sugg[3]; Weizhou Zhang[3]; Weiguo Andy Tao[1]; *[1]Purdue University, West Lafayette, IN; [2]Tymora Analytical Operations, West Lafayette, IN; [3]University of Iowa, Iowa City, Iowa*

WP 121 **Multiplexed Measurement of Catecholamines in the Serum and Urine of Non-Human Primates Utilizing Sample Derivatization and UPLC-MS/MS**; Kimberly A Navetta[1]; Rebecca R Ferreira[1]; Mireia Fernandez Ocana[1]; *[1]Pfizer Inc., Andover, MA*

WP 122 **Rapid Diagnosis of Infectious Disease by Quantification of a Circulating Antigen**; Jia Fan[1]; Ye Hu[1]; *[1]Arizona State University, Tempe, AZ*

WP 123 **Validating Mass Spectrometry Platforms for Profiling of Aberrant IgA1 O-Glycosylation Implicated in Pathogenesis of IgA Vasculitis with Nephritis**; Alyssa L. Hansen[1]; Audra A. Hargett[1]; Ellenore P. Craine[1]; Stacy Hall[1]; Bruce A. Julian[1]; Jan Novak[1]; Matthew B. Renfrow[1]; *[1]University of Alabama at Birmingham, Birmingham, Alabama*

WP 124 **Development of an Automated LC-MS Based Assay Using a SISCAPA Workflow to Enable Quantitation of Peptide Biomarkers of Neurodegeneration**; Julie Lee[1]; Paul L Auger[1]; Kristin Wildsmith[1]; *[1]Genentech Inc., South San Francisco, CA*

WP 125 **Development of a Fit-for-Purpose LC-MRM-MS assay to measure Prion Protein in Cerebrospinal Fluid**; Alexandra R Cocco[1]; Eric Kuhn[1]; Eric Vallabh Minikel[1]; Christina R Hartigan[2]; Sonia M Vallabh[1]; Stuart L Schreiber[1]; Steven A Carr[1]; *[1]Broad Institute of MIT and Harvard, Cambridge, MA; [2]Emory University, Atlanta, GA*

WP 126 **Developing an Automated Plasma Sample Preparation Method for LC/MS Analysis of Metabolites**; Koen Raedschelders[1]; Weston Spivia[1]; Jennifer Van Eyk[1]; *[1]Cedars-Sinai Medical Center, Los Angeles, CA*

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WP 127 **Evaluating the Efficiency of DSS Cross-Linking Reaction in Different Conditions and the Correlation between Obtained Distance Constraints and Crystallographic Structure**; Bruno C Amaral[1]; Fabio Cesar Gozzo[1]; *[1]Dalton Mass Spectrometry Laboratory, Institute of Chemistry, University of Campinas, Campinas, Brazil*

WP 128 **Protein Footprinting Method Coupled with Mass Spectrometry for the Structural Analysis of Cystic Fibrosis Transmembrane Conductance Regulator**; Zhihui Zhang[1]; Lisa M Jones[2]; *[1]University of Maryland, Baltimore, Baltimore, MD; [2]University of Maryland Baltimore, Baltimore, MD*

WP 129 **Innovation Assembly, and Optimization of a Novel Pulse-Chase In Cell Footprinting Method for the Study of Protein Folding**; Dante T Johnson[1]; Ben Punshon-Smith[2]; Anne Gershenson[3]; Lisa M Jones[1]; *[1]University of Maryland Baltimore School of Pharmacy, Baltimore, MD; [2]University of Maryland Baltimore County, Baltimore, MD; [3]University of Massachusetts Amherst, Amherst, MA*

WP 130 **Extension of Fast Photochemical Oxidation of Proteins for *in vivo* Modification in Caenorhabditis elegans**; Jessica A Espino[1]; Zhihui Zhang[1]; Lisa M Jones[1]; *[1]University of Maryland Baltimore School of Pharmacy, Baltimore, MD*

WP 131 **Covalent Labeling is Sensitive to Residue Microenvironment, Providing Improved Structural Analysis of Protein Higher Order Structure**; Patanachai Limpikirati[1]; Xiao Pan[1]; Richard W. Vachet[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

WP 132 **Quantification of Differentially Crosslinked Proteins and Peptides**; Billy Samulak; *Fitchburg State University, Fitchburg, Massachusetts*

WP 133 **A Synthetic Crosslinked Peptide Library for Benchmarking Algorithms Developed for Crosslink Identification**; Rebecca Beveridge[1]; Johannes Stadlmann[2]; Karl Mechtler[1,2]; *[1]Research Institute of Molecular Pathology, Vienna, Austria; [2]Institute of Molecular Biotechnology, Vienna, Austria*

WP 134 **Monitoring of hSCN Binding-Site Using Multiple MS-Based Methods**; Chunyang Guo[1]; Lindsey Steinberg[2]; Ming Cheng[1]; Jing Yan[1]; Jeffrey P Henderson[2]; Michael L Gross[1]; *[1]Department of Chemistry, Washington University in St Louis, St Louis, MO; [2]Division of Infectious Diseases, Department of Medicine, Washington University School of Medicine, St Louis, Missouri*

WP 135 **On-line Miniaturized Asymmetrical Flow Field-Flow Fractionation Separation with Fast Photochemical Oxidation of Proteins (FPOP)**; Jong Hee Song[1]; Don L Rempel[1]; Michael L Gross[1]; *[1]Washington University in St. Louis, St. Louis*

WP 136 **Accommodating Ambiguity in Crosslink Detection for Applications in Integrative Structural Modeling**; Andrew RG Michael[1]; Wei Yang[1]; Daniel S Ziemianowicz[1]; David C Schriemer[1]; *[1]University of Calgary, Calgary, AB*

WP 137 **Developing Tris(hydroxymethyl)aminomethane as an UV-Active Hydroxyl Radical Dosimeter**; Addison E Roush[1]; Mohammad Riaz[1]; Sandeep K Misra[1]; Joshua S Sharp[1]; *[1]University of Mississippi Department of Biomolecular Sciences, University, MS*

WP 138 ***In situ* Production of Hydroxyl Radicals by Ozone from Laser Photolysis of Solvated Oxygen at Physiological pH for Protein Footprinting**; Simin D. Maleknia[1]; Callan Wilcox[2]; Scott Kable[2]; *[1]University of Technology Sydney, Sydney, Australia; [2]School of Chemistry, University of New South Wales, Sydney, NSW, Australia*

WP 139 **Oxidation Effects on Chymotrypsin Digested HRPF Samples and Observation of Highly Basic Regions**; Charles Mobley[1]; Niloofar Abolhasani Khaje[1]; Pradeep Prabhakar[2]; Kelley Moremen[2]; Joshua S. Sharp[1]; *[1]University of Mississippi, University, MS; [2]University of Georgia, Athens, GA*

WP 140 **Sub-Residue Resolution Footprinting of Ligand-Protein Interactions Enabled by Ion Mobility Mass Spectrometry**; Gaoyuan Lu[1]; Nian Wang[1]; Yang Tian[1]; Ning Wan[1]; Yatao Shi[2]; Gongyu Li[2]; Lingjun Li[2]; Haiping Hao[1]; Hui Ye[1]; *[1]China Pharmaceutical University, Nanjing, Jiangsu, China; [2]University of Wisconsin - Madison, madison*

WP 141 **Uncovering the Molecular Architecture of Human Fibrin Clots by Crosslinking Mass Spectrometry**; Oleg Klykov[1,2]; Carmen van der zwaan[3]; Alexander B. Meijer[3]; Albert J.R. Heck[1,2]; Richard A. Scheltema[1,2]; *[1]Utrecht University, Utrecht, Netherlands; [2]Netherlands Proteomics Center, Utrecht, Netherlands; [3]Sanquin Research, Amsterdam, Netherlands*

WP 142 **Mechanistic Studies of Radical Trifluoromethylation and its Application for Membrane Protein Labeling and Epitope Mapping**; Ming Cheng[1]; Chunyang Guo[1]; George Mathai[2]; Gary Gerstenecker[1]; Don Rempel[1]; Michael L. Gross[1]; *[1]Washington University, St.louis, MO; [2]Sacred Heart College, Cochin, India*

WP 143 **In-Cell Fast Photochemical Oxidation of HCT116 Spheroids**; Raquel Shortt[1]; Jesica Lukowski[2]; Amanda B. Hummon[3]; Lisa M Jones[1]; *[1]University of Maryland Balitmore, Baltimore, MD; [2]University of Notre Dame, Notre Dame, IN; [3]The Ohio State University, Columbus, OH*

WP 144 **Evaluation of FAIMS Technology for Mass Spec Analysis of Chemical Cross-Linked Peptides**; Rosa Viner[1]; Leigh A Foster[2]; Ryan D. Bomgarden[2]; Michael W. Belford[1]; Satendra Prasad[1]; Romain Huguet[1]; Eloy R. Wouters[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]ThermoFisher Scientific, Rockford, IL*

WP 145 **Photo Affinity Fragment (PhABit) Screening: A High Throughput Assay Platform and Identification of PhABit Binding Sites**; Chad J Quinn[1]; Ken Fantom[2]; Craig Wagner[1]; Emma Grant[2]; Jacob Bush[2]; Chun-wa Chung[2]; Mike Hann[2]; Roland S Annan[1]; Francesca Zappacosta[1]; *[1]GSK, Collegeville, PA; [2]GSK, Stevenage, United Kingdom*

WP 146 **Mass Spectrometry-Based Protein Footprinting Reveals Conformational Dynamics of the Plasma Membrane Proton Pump**; Thao T. Nguyen[1]; Pei Liu[2]; Benjamin Minkoff[1]; Michael Sussman[1]; *[1]UW Madison, Madison, WI; [2]University of Missouri, Columbia, MO*

WP 147 **Measuring Protein Conformational Change in living Cells by Quantitative, Comprehensive, and Ultra-Sensitive Protein Footprinting**; Jenna G. Caldwell[1]; Joshua E. Elias[2]; Pehr A. B. Harbury[2]; *[1]Stanford University, Stanford, CA; [2]Stanford University, Palo Alto, CA*

WP 148 **Developing an Integrative XL-MS Strategy to Facilitate Structural Modeling of Protein Complexes**; Craig B Gutierrez[1]; Ilan Chemmama[2]; Haibin Mao[3]; Clinton Yu[1]; Sara Block[1]; Scott Rychnovsky[1]; Ning Zheng[3]; Andrej Sali[2]; Lan Huang[1]; *[1]University of California, Irvine, Irvine, CA;*

[2]University of California at San Francisco, San Francisco, CA; [3]University of Washington, Seattle, WA

WP 149 **Novel Reagent Efficiently Esterifies Hydroxyl-Containing Amino Acids and Provides Promise as a Covalent Protein Footprinter**; Austin B Moyle[1]; Ming Cheng[1]; Nicole D Wagner[1]; Michael L Gross[1]; [1]Washington University in St. Louis, St. Louis, MO

WP 150 **Specific Identification of Dityrosine cross-linked Peptides using 193 nm Ultraviolet Photodissociation Mass Spectrometry**; Soumya Mukherjee[1]; Mengxuan Fang[2]; W. Mei Kok[3]; Eugene Kapp[1]; Craig A. Hutton[2, 3]; Gavin Reid[2, 3]; Blaine Roberts[1]; [1]The Florey Institute of Neuroscience and Mental Health, The University of Melbourne, Melbourne, Australia; [2]School of Chemistry, Bio21 Molecular Science and Biotechnology Institute, The University of Melbourne, Parkville, 3010, Melbourne, Australia; [3]Department of Biochemistry and Molecular Biology, The University of Melbourne, Parkville, Victoria, 3010, Melbourne, Australia

WP 151 **Assessing the Conformation of Influenza Hemagglutinins Using Covalent Labeling and Intact Mass Spectrometry Approaches**; Jonathan Bundy[1]; Carrie L. Pierce[1]; Dongxia Wang[1]; Jakub Baudys[1]; Tracie L Williams[1]; John R. Barr[1]; [1]CDC, Atlanta, GA

WP 152 **Structure-Function Relationship of Cyanobacterial Flavodiiron Proteins Revealed by Combined Approaches of in Solution and Computational Methods**; Monika Tokmina-Lukaszewska[1]; Katherine A Brown[2]; Zhanjun Guo[2]; Liam W Scott[1, 3]; Carolyn E Lubner[2]; Sharon Smolinski[2]; David W Mulder[2]; Brian Bothner[1]; Paul W King[2]; [1]Montana State University, Bozeman, MT; [2]National Renewable Energy Laboratory, Golden, CO; [3]Indiana University, Bloomington, IN

WP 153 **Measurement of Enthalpies of Ubiquitin Dimerization to Different Dimer Structures**; Bingqing Zhao[1]; Colin P. Reilly[1]; James P. Reilly[1]; [1]Indiana University, Bloomington, IN

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WP 154 **A Multiresidue Approach to Pesticide Screening in Cannabis Using GC-MS/MS**; Kari Organtini[1]; Kim Tran[1]; Kenneth Rosnack[1]; Peter Hancock[2]; Naren Meruva[1]; [1]Waters Corporation, Milford, MA; [2]Waters Corporation, Wilmslow, United Kingdom

WP 155 **From Cigarettes to Joints - Puff-by-Puff Resolved Analysis of Smoke Constituents of Cannabis Products Other Smoking Devices Using Photoionization TOF-MS**; Sven Ehlert[1]; Jan Heide[2]; Andreas Walte[1]; Mohammad Saraji-Bozorgzad[1]; Matthias Bente v Frowein[1]; Ralf Zimmermann[2]; [1]Photonion GmbH, Schwerin, Germany; [2]University of Rostock, Rostock, Germany

WP 156 **Determination of Pesticides and Mycotoxins in Cannabis Using a Simple Extraction Procedure with dSPE Cleanup and LC-MS/MS**; Kim Tran[1]; Marian Twohig[1]; Kari Organtini[1]; Michael S. Young[1]; Naren Meruva[1]; Kenneth Rosnack[1]; Rebecca Stevens[2]; James Roush[2]; Chris Hudalla[2]; Sarah Dowd[3]; Gordon Fujimoto[3]; [1]Waters Corporation, Milford, MA; [2]Proverde Laboratories, Milford, MA; [3]Waters Corporation, Beverly, MA

WP 157 **A Novel LCMSMS Method with Dual ESI and APCI Source for Analysis of Pesticides in Cannabis Flower**; Avinash Dalmia[1]; Erasmus Cudjoe[2]; Jacob Jalali[3]; Jingcun Wu[2]; Josh Ye[2]; Heather Gamble[2]; Reza Javahery[2]; Feng Qin[2]; [1]Perkinelmer, Shelton, CT; [2]PerkinElmer, Woodbridge, ON; [3]Perkin Elmer, San Jose, CA

WP 158 **Rapid Multipexed Analysis of Cannabinoids and their Metabolites in Urine Using MassHunter StreamSelect LC-MS System**; Andre Szczesniewski[1]; Kevin McCann[1]; [1]Agilent Technologies, Wood Dale, IL

WP 159 **Simplified Sample Preparation for Low Level Determination of Cannabis Use from Hair Samples Prior to LC-MS/MS Analysis**; Katie-Jo Teehan[1]; Lee Williams[1]; Rhys Jones[1]; Adam Senior[1]; Helen Lodder[1]; Geoff Davies[1]; Alan Edgington[1]; Steve Jordan[1]; Claire Desbrow[1]; Paul Roberts[1]; [1]Biotage GB Limited, Cardiff, United Kingdom

WP 160 **Quantitation of California Regulated Pesticides in Cannabis Oil by ESI/APCI UHPLC-MS-MS**; Jacob Jalali[1]; Avinash Dalmia[2]; Erasmus Cudjoe[3]; Feng Qin[3]; Jingcun wu[3]; Luke Ward[4]; Ben Armestrong[4]; [1]PerkinElmer, San Jose, CA; [2]PerkinElmer, Shelton , CT; [3]PerkinElmer, Woodbridge, ON; [4]Juniper Analytics, Bend, OR

WP 161 **Similarities and Differences in the Fragmentation Pathways of Cannabinoid Ions Generated by Electron Impact, Electrospray Ionization, Atmospheric Pressure Chemical Ionization**; Allegra Leghissa[1]; Zacariah L. Hildenbrand[2]; Kevin A Schug[3]; [1]University of Texas, Arlington, Arlington, TX; [2]Inform Environmental LLC., Dallas, Texas; [3]University of Texas Arlington, Arlington

WP 162 **A Draft Map of the Cannabis Proteome**; Benjamin Orsburn[1]; Conor Jenkins[1, 2]; [1]Think20 Labs, Columbia, MD; [2]Hood College Bioinformatics Program, Frederick, MD

WP 163 **High Throughput Testing of Terpenes in Cannabis Samples by Headspace/Gas Chromatography/ Mass Spectrometry**; Adam Floyd[1]; Adam Patkin[1]; Lee Marotta[1]; Charlie Schmidt[2]; [1]Perkin Elmer, San Jose, CA; [2]PerkinElmer, San Jose, CA

WP 164 **Streamlining Cannabis Testing using Comprehensive Two-Dimensional Gas Chromatography with Time-of-Flight Mass Spectrometry (GCxGC-TOFMS)**; Joseph E Binkley[1]; Brad Barrett[2]; David E Alonso[2]; [1]LECO Corporation, St. Joseph, MI; [2]LECO Corporation, St Joseph, MI

WP 165 **Evaluating Cannabinoids and Terpenes in Challenging Matrices Using High-Temperature Headspace-Gas Chromatography-Mass Spectrometry**; Don Nguyen[1, 2]; Seamus Riordan-Short[1]; Thu-Thuy Dang[2]; Rob O'Brien[1]; Matthew Noestheden[1]; [1]Supra R&D, Kelowna, BC; [2]University of British Columbia, Kelowna, British Columbia

WP 166 **Comprehensive Untargeted Screening and Quantitation of Pesticides in Cannabis Using GCxGC and High Performance Time of Flight Mass Spectrometry**; Gail Harkey[1]; Todd Richards[1]; Joseph E Binkley[2]; David E Alonso[1]; Lorne Fell[1]; [1]LECO Corporation, St Joseph, MI; [2]LECO Corporation, St. Joseph, MI

WP 167 **Does Your Dog Have Anxiety After a Rough Day at the Lake: Analysis of CBD Extracts for Dog Treats**; Matthew Curtis[1]; Mike Adams[2]; Karen Kaikaris[2]; Sarah Aijaz[3]; Sue D'Antonio[1]; Anthony Macherone[1, 4]; [1]Agilent Technologies, Inc., Santa Clara, CA; [2]CWC Labs, Cedar Creek, TX; [3]MilliporeSigma, Bellefonte, PA; [4]Johns Hopkins University School of Medicine, Baltimore, MD

WP 168 **Time Saving Sample Prep for the Analysis of 54 Residues in Cannabis Flower by LC-MS/MS**; Lisa Wanders; Thomson Instrument Co, Oceanside, CA

WP 169 **MALDI-MS Library of Fingerprint Spectra for Selected Fractions of Cannabis Products**; Baylie Gigolyk[1]; Helene Perreault[1]; [1]University of Manitoba, Winnipeg, MB

WP 170 **An Automated LC-MS/MS Workflow for High-Throughput Pesticide Residue Screening in Cannabis Samples**; Mahsan Miladi[1]; Tanner Stevenson[1]; [1]Agilent Technologies, Santa Clara, CA

WP 171 **The Analysis of Mycotoxins in CBD Oils by LC-MS/MS**; Justin Steimling[1]; Megan Pollock[1]; Ty Kahler[1]; Colton Myers[1]; Ashlee Reese[1]; Susan Steinike[1]; [1]Restek, Bellefonte, PA

WP 172 **Method Development and Validation for Liquid Chromatography/Tandem Mass Spectrometry Determination of Cannabidiol, Tetrahydrocannabinol, and Metabolites in Equine Urine and Plasma**; Michael

Hedge[1]; Nathan Mitchell[1]; Scott Stanley[1,2]; Rui Yu[1]; *[1]United States Equestrian Federation Equine Drug Testing and Research Laboratory, Lexington, KY; [2]University of Kentucky, Lexington, KY*

WP 173 **Screening CBD Oil Pet Supplements for Mycotoxins using LC-MS Quadrupole System with Accurate Mass Calibration**; Sue D'Antonio[1]; Yongdong Wang[2]; Don Kuehl[2]; Anthony Macherone[3,4]; *[1]Agilent Technologies, Inc., Santa Clara, CA; [2]Cerno Bioscience LLC, Norwalk, CT; [3]Agilent Technologies, Wilmington, DE; [4]Johns Hopkins University School of Medicine, Baltimore, MD*

WP 174 **When Matrix Matched Calibration Systems Don't Match Truth: Distinguishing Trueness from Accuracy for THC-COOH in Urine**; Matthew T Campbell[1]; Kyle Cahill[1]; Brian Rappold[1]; *[1]LabCorp, Research Triangle Park, NC*

WP 175 **Solvent-Free Terpene & Cannabinoid Profiling of Cannabis and Cannabis-Infused Consumer Products using Vacuum Assisted Sorbent Extraction (VASE) Thermal Desorption-GC-MS**; Sage J.B. Dunham[1]; Victoria L. Noad[1]; Daniel B. Cardin[1]; *[1]Entech Instruments Inc, Simi Valley, CA*

WP 176 **Analogue and Digital 1 Hz Infusion SCREENING of Mixtures via IBF Droplets**; Drew Sauter[1]; Ron Shomo[2]; *[1]Nanoliter, LLC, Henderson, NV; [2]Scientific Instrument Services, Ringoes, NJ*

WP 177 **Liquid Chromatography and Tandem Mass Spectrometry: The Technique for Analyzing Pesticides in Cannabis Flower to Meet Regulatory Requirements in Canada**; Erasmus Cudjoe[1]; Dalmia Avinash[2]; Jacob Jalali[3]; Jingcun Wu[4]; Josh Ye[5]; Feng Qin[5]; *[1]PerkinElmer, Canada, Woodbridge, ON; [2]Perkinelmer, Shelton, CT; [3]Perkin Elmer, San Jose, CA; [4]PerkinElmer, Inc.,, Woodbridge, ON; [5]PerkinElmer Inc., Woodbridge, ON*

WP 178 **LC-MS/MS Dilute and Shoot Development and Validation for the Quantitation of 11-Nor-9-Carboxy-THC and Cannabidiol in Urine**; Chris Riley[1]; Lawrence J Andrade[1]; *[1]Dominion Diagnostics, North Kingstown, RI*

WP 179 **GC/MS and HPLC/MS Characterization of the Terpenes, Sesquiterpenes and Cannabinoids in Cannabis and Cannabis Products**; Jodie V Johnson[1]; Kari B. Green[1]; Adam Christensen[2]; Daniel Morgan[2]; *[1]Chemistry Dept, University of Florida, Gainesville, FL; [2]Botanica Testing LLC, Gainesville, FL*

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WP 180 **Resolving the Isomeric Heterogeneity of the Glycome: Ultrahigh-Resolution Ion Mobility Separations in Structures for Lossless Ion Manipulations**; Gabe Nagy[1]; Isaac K. Attah[1]; Sandilya V. B. Garimella[1]; Yehia M. Ibrahim[1]; Richard D. Smith[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

WP 181 **Quantitative Glycomics with Improved Multiplexing Performance by Mass-Defect SUGAR Tags and Both-ends Labeling**; Miyang Li[1]; Yu Feng[2]; Lingjun Li[1,2]; *[1]Department of Chemistry, University of Wisconsin, Madison, WI; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI*

WP 182 **Introduction of a Novel Labelling Strategy to Facilitate LC-MS Analysis of Released N-Glycans**; Phil J Widdowson[1]; Zoltan Szabo[2]; Sheheer Khan[2]; Jonathan Bones[3]; Rowan Moore[4]; *[1]Thermo Fisher Scientific, Runcorn, United Kingdom; [2]Thermo Fisher Scientific, Oyster Point, California; [3]National Institute for Bioprocessing Research and Training, Dublin, Ireland; [4]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom*

WP 183 **Structural Analysis of Free Oligosaccharides from Bovine Milk with New Mass Spectrometry Method**; Chi-kung Ni[1]; WeiChien Weng[2]; Hsu-Chen Hsu[1]; Shang-Ting Tsai[1]; Chia Yen Liew[1]; Shih-Pei Huang[1]; Yu-Shiang Kuo[1]; *[1]Academia Sinica, Taipei, Taiwan; [2]Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei City, Taiwan*

WP 184 **Harmonization of Glycan Structure Identification for Translational Human Cardiac Glycomics**; Christopher Ashwood[1]; Matthew Waas[1]; Ranjuna Weerasekera[1]; Rebekah L. Gundry[1]; *[1]Medical College of Wisconsin, Milwaukee, WI*

WP 185 **Ion Pairing Effects in Carbohydrate Ion-Electron Reactions**; Isaac Agyekum[1]; Kristina Hakansson[1]; *[1]University of Michigan, Ann Arbor, MI*

WP 186 **Avian IgY N-linked Glycan Structural Determination Using Ion Trap Mass Spectrometry**; Kate Stumpo[1]; Kevin Kover[1]; Robert Smith[1]; Margret Hatch[2]; David Ashline[3]; Vernon Reinhold[3]; *[1]University of Scranton, Scranton, PA; [2]Penn State University - Scranton, Dunmore, PA; [3]University of New Hampshire, Durham, NH*

WP 187 **The Quantification of Chondroitin Sulfate in Raw Materials and Dietary Supplements**; Martina Hermannova[1]; Daniela Smejkalova[1]; Tomas Bobula[1]; *[1]Contipro a.s., Dolni Dobrouc, Czech Republic*

WP 188 **Structural Characterization of Oligosaccharide Mixtures Using Ultra-High Performance Liquid Chromatography (UHPLC) with Charge Transfer Dissociation Mass Spectrometry (CTD-MS)**; Praneeth M. Mendis[1]; Zachary J. Sasiene[1]; David Ropartz[2]; Helene Rogniaux[2]; Glen P. Jackson[1,3]; *[1]C. Eugene Bennett Department of Chemistry, West Virginia University, Morgantown, WV; [2]INRA UR1268 BIA, Nantes, France; [3]Department of Forensic and Investigative Science, West Virginia University, Morgantown, WV*

WP 189 **Characterization of Enoxaparin using LC-MS/MS**; S Sameer Kumar Gantasala[1]; Dilipkumar Reddy Kandula[2]; Sri Rama Krishna Surapureddi[1]; Sreedhar Reddy Sappidi[1]; Manoj Pillai[2]; Shrikrishna Dadke[1]; *[1]Vimta Labs Limited, Hyderabad, India; [2]SCIEX INDIA, GURUGRAM, India*

WP 190 **Sequencing Heparan Sulfate Using Liquid Chromatography Tandem Mass Spectrometry**; Jiandong Wu[1]; Juan Wei[1]; Pradeep Chopra[2]; Geert-Jan Boons[2,3]; Cheng Lin[1]; Joseph Zaia[1]; *[1]Boston University, Boston, MA; [2]University of Georgia, Athens, GA; [3]Utrecht Univeristy, Utrecht, Netherlands*

WP 191 **A New Method for the Analysis of Bisecting N-Glycans on the Intact Glycopeptides**; Liuyi Dang[1]; Jiechen Shen[1]; Shisheng Sun[1]; *[1]Northwest University, Xi'an, China*

WP 192 **New Method for Highly Sensitive Analysis of Complex Oligosaccharides Based on Filter Aided Sample Preparation and Mass Spectrometry**; Amandine Pruvost[1]; Christophe Penverne[1]; Christian Rolando[1]; *[1]Université de Lille, Villeneuve d'Ascq, France*

WP 193 **Investigating Isoform Structures Found In Enoxaparin Using Negative Electron Transfer Dissociation And Capillary Electrophoresis-Mass Spectrometry**; Morgan Stickney[1]; Patience Sanderson[1]; Franklin E. Leach Iii[1]; Joshua J Coon[2]; Michael S Westphall[2]; Nicholas M Riley[2]; Qiangwei Xia[3]; Robert Linhardt[4]; I. Jonathan Amster[1]; *[1]University of Georgia, Athens, GA; [2]University of Wisconsin-Madison, Madison, WI; [3]CMP Scientific Corp, New York, NY; [4]Rensselaer Polytechnic Institute, Troy, NY*

WP 194 **A Novel Isobaric Tag Enabled Multiplexed Quantitative Glycomics Analysis for Various Types of N-glycans including Sialic Acid Linkage Isomers**; Qinying Yu[1]; Yu Feng[1]; Lingjun Li[1]; *[1]University of Wisconsin Madison, Madison*

WP 195 **The Unexpected Dissociation Mechanism of Sodiated N-acetylglucosamine and N-acetylgalactosamine**; Shih-Pei Huang[1]; Shang-Ting Tsai[1]; Hou-Yu Lin[1,2]; Chi-Kung Ni[1]; *[1]Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei, Taiwan; [2]Department of Chemistry, National Taiwan University, Taipei, Taiwan*

WP 196 **Investigation on Isomeric Gangliosides using LC/MS/MS towards Mouse Brain Regional Mapping**; Jua Lee[1]; Jaekyung Yun[1]; Heeyoun Hwang[1]; Hee-sup Shin[2]; Hyun Joo An[1]; *[1]Chungnam National University, Daejeon, South Korea; [2]Institute for basic science, Daejeon, South Korea*

WP 197 **Isomeric Separation of Permethylated Glycans by Extra-Long Reversed-Phase Liquid Chromatography (RPLC)-MS**; Xue Dong[1]; Yifan Huang[1]; Jingfu Zhao[1]; Aiying Yu[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

WP 198 **Discrimination of Metal Adducted Sialylated Carbohydrate Isomers by Ion Mobility Spectrometry, Electron Transfer, and Vibrational Activation**; Anna J. Diepenbrock[1]; Eric D. Dodds[1]; *[1]University of Nebraska - Lincoln, Lincoln, NE*

WP 199 **Degradation Pathway of β-Cyclodextrin by Electrospray Ionization Mass Spectrometry and Liquid Chromatography with Evaporative Light Scattering Detection**; Hengwen Zhong[1]; Peter Wang[1]; Tao Jiang[1]; *[1]Mallinckrodt, Hazelwood, MO*

WP 200 **Characterization of Sodium and Lithium Cationized Mono and Disaccharides Using High Resolution IMS and Tandem IMS Techniques**; Paul Scott Soma[1]; Matthew T Campbell[1]; Andrew Baker[2]; Martin Palmer[3]; Dale Cooper-Shepherd[3]; Gary Glish[1]; *[1]University of North Carolina, Chapel Hill, NC; [2]Waters Corporation, Pleasanton, CA; [3]Waters, Wilmslow, United Kingdom*

WP 201 **Determining the Structure of the Glycan Bearing the Bisecting GlcNAc on Human Placenta Membrane Using Mass Spectrometry**; Qiushi Chen[1]; Yuanliang Zhang[1]; Zhilong Lin[1]; Yan Ren[1]; Siqi Liu[1]; *[1]BGI-Shenzhen, Beishan Industrial Zone 11th Building, Yantian District, Shenzhen City, China*

WP 202 **A Facile and Unbiased Method for Comprehensive Glycome Characterization**; Juan Wei[1]; Yang Tang[2]; Pengyu Hong[3]; Catherine E. Costello[1,2]; Cheng Lin[1]; *[1]Department of Biochemistry, Boston University School of Medicine, Boston, MA; [2]Department of Chemistry, Boston University, Boston, MA; [3]Department of Computer Science, Brandeis University, Waltham, MA*

WP 203 **Isoforms of Carbohydrates Identified by 2D UV-MS of Non-Covalent Complexes with Aromatics**; Oleg V. Boyarkine; *EPFL, Lausanne, Switzerland*

WP 204 **Separation and Identification of Glycan Anomers Using Ultrahigh-Resolution Ion Mobility Spectrometry Combined with Cryogenic IR Spectroscopy**; Stephan Warnke[1]; Ahmed Ben Faleh[1]; Thomas R. Rizzo[1]; *[1]Ecole Polytechnique Federale de Lausanne, Lausanne, Switzerland*

WP 205 **Dual Enzymatic Digestion Enabling Simultaneous Release of Glycans from Glycoproteins and Glycolipids**; Seth D Williamson[1]; Andrew Cho[1]; Jair Montford[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

CLINICAL ANALYSIS III
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WP 206 **Noninvasive Analysis and Delivery of Vitamin D3 in the Skin**; Isaac Mall[1]; Marcel Musteata[1]; *[1]Albany College of Pharmacy, Albany, NY*

WP 207 **An Ultra-Sensitive Paper-Based Diagnostic Platform of Detecting Colorectal Cancer via Mass Spectrometry**; Suji Lee[1]; Abraham K. Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH*

WP 208 **Rapid, Robust and High-Throughput Proteome Analysis by High-Flow LC-MS/MS**; Yangyang Bian[1]; Runsheng Zheng[1]; Yun-Chien Chang[1]; Jana Zecha[1]; Stephanie Heinzlmeir[1]; Daniel P Zolg[1]; Oleksandr Boichenko[2]; Mike Baynham[3]; Bernhard Kuster[1,4,5]; *[1]Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; [2]Thermo Fisher Scientific, Germering, Germany; [3]Thermo Fisher Scientific, Runcorn, United Kingdom; [4]Center for Integrated Protein Science Munich, Freising, Germany; [5]Bavarian Center for Biomolecular Mass Spectrometry, Freising, Germany*

WP 209 **A High Throughput and High Resolution LC-MS/MS Method to Measure IGF1 in Serum for Clinical Research**; Xiaolei Xie; *ThermoFisher Scientific, San Jose, CA*

WP 210 **Faecal Metabolomics by Conventional UHPLC-HRMS as well as Novel LA-REIMS Reveals Relevant Metabolic Perturbations in Type 2 Diabetes**; Lieven Van Meulebroek[1]; Simon Cameron[2]; Bruno Lapauw[3]; Zoltan Takats[2]; Lynn Vanhaecke[1]; *[1]Ghent University, Merelbeke, Belgium; [2]Imperial College, London, United Kingdom; [3]Ghent University Hospital, Ghent, Belgium*

WP 211 **Clinical Evaluation of Coated Blade Spray Mass Spectrometry for the Concomitant Determination of Four Immunosuppressive Drugs in Whole Human Blood**; Daniel Rickert[1]; German Augusto Gomez-Rios[1,2]; Emir Nazdrajić[1]; Marcos Tascon[1,3]; Vathany Kulasingam[4,5]; Janusz Pawliszyn[1]; *[1]University of Waterloo, Waterloo, ON; [2]Restek Corporation, Bellefonte, PA; [3]Instituto de Investigación e Ingenieria Ambiental (3iA), Universidad Nacional de San Martín (UNSAM), San Martín, Argentina; [4]Department of Laboratory Medicine and Pathobiology, University of Toronto, Toronto, Ontario; [5]Department of Clinical Biochemistry, University Health Network, Toronto, Ontario*

WP 212 **An Approach to Screening Clinical Samples for Novel Fentanyls using High Resolution Tandem Mass Spectrometry**; Kenneth D. Swanson[1]; Rebecca L. Shaner[1]; William A. Bragg[1]; Logan C. Krajewski[2]; Elizabeth I. Hamelin[1]; Melissa D. Carter[1]; Rudolph C. Johnson[1]; *[1]Emergency Response Branch, Division of Laboratory Sciences, National Center for Environmental Health, Centers for Disease Control and Prevention, Atlanta, GA; [2]Battelle Memorial Institute at the Centers for Disease Control and Prevention, Atlanta, GA*

WP 213 **Different Approaches for Vitamin D Determination in Newborns by LC-MS/MS**; Rafal Rola[1,2]; Konrad Kowalski[2]; Tomasz Bienkowski[2]; Jacek Witwicki[3]; *[1]Nicolaus Copernicus University, Torun, Poland; [2]Masdiag Sp. z o.o., Warsaw, Poland; [3]Bielanski Hospital, Warsaw, Poland*

WP 214 **A Simple Analysis of Catecholamines in Cell Cultures by LC/MS/MS Using an Ion-Pairing Reagent Added to Final Extracts**; Yi Zhao[1]; Peiling Hou[2]; Shu Qing Chan[3]; Weiying Sim[1]; Lisa Helen Ong[1]; Jie Xing[2]; *[1]Department of Clinical Research, Singapore General Hospital,, Outram Road, Singapore; [2]Application Development & Support Centre, Shimadzu (Asia Pacific) Pte Ltd, Singapore; [3]School of Chemical and Life Sciences, Singapore Polytechnic, Singapore*

WP 215 **Application of the HPLC-MS/MS Method in Studying Individual Metabolic Differences of Cyclosporin A in Bone Marrow Transplant Patients**; Wang Lei[1,2]; Liu hong xing[2,3,4]; Liu rui[1]; Yang zi yi[1]; *[1]HebeiYanda Lu Daopei Hospital, Langfang, China; [2]Beijing Lu Daopei Hospital, Beijing, China; [3]HebeiYanda Lu Daopei Hospita, Langfang, China; [4]Beijing Lu Daopei Institute of Hematology, Beijing, China*

WP 216 **Intra-Surgical Diagnosis of IDH Mutation in Human Glioma using a Miniature Mass Spectrometer**; Fan Pu[1]; Clint M Alfaro[1]; Hannah M Brown[1]; Zheng Ouyang[1,2]; Graham R. Cooks[1]; *[1]Department of Chemistry, Purdue University, West Lafayette, IN 47907; [2]Tsinghua University, Beijing, China*

WP 217 **High-Throughput Analysis of Neuroleptic Drugs in Plasmas using LDTD-MS/MS Technology**; Jacques Corbeil[1,2]; Serge Auger[3]; Pier-Luc Plante[1,2]; Jean Lacoursière[3]; Pierre Picard[3]; *[1]Université Laval, Quebec, Quebec; [2]Infectiology Research Centre, CHU de Québec, Laval University, Québec, QC; [3]Phytronix Technologies, Quebec, QC*

WP 218 **Reliable Quantification of 52 Amino Acids in Human Plasma by LC-MS/MS**; Stephanie Samra[1]; Valérie Thibert[2]; Claude Netter[2]; [1]*Thermo Fisher Scientific, San Jose, CA;* [2]*Thermo Fisher Scientific, Courtaboeuf, France*

WP 219 **High-Sensitivity Analysis of a Steroid Panel Samples using Micro-Flow LC-MS/MS for Clinical Research**; Narumi Shirai[1]; Takanari Hattori[2]; Mikael Levi[2]; Shoji F. Nakayama[3]; Shigeru Suzuki[1]; [1]*Chubu University, Kasugai, Japan;* [2]*Shimadzu Corporation, Kyoto, Japan;* [3]*National Institute for Environmental Studies, Tsukuba, Japan*

WP 220 **Using Superficially Porous Phenyl Phase Selectivity for Benzodiazepine Separations**; William Long[1]; Carl Griffin[2]; Anne E Mack[2]; Emily Parry[2]; Charles Lofton[2]; [1]*Agilent Technologies, Wilmington, DE;* [2]*Agilent Technologies, Inc., Wilmington, DE*

WP 221 **A Systematic Study of Hydrolytic Degradation of Acylcarnitines During Sample Preparation and Analysis in Newborn Screening Using Tandem Mass Spectrometry**; Timothy Lim[1]; Donald H Chace[1]; Konstantinos Petritis[1]; [1]*Centers for Disease Control and Prevention, Chamblee, GA*

WP 222 **Translation of a Top-Down Proteomics IgG Workflow to the Mayo Clinic to Characterize Monoclonal Gammopathies**; Ryan T Fellers[1]; Richard D Leduc[1]; Bryan P Early[1]; Rafael D. Melani[1]; Joseph B Greer[1]; Surendra Dasari[2]; Patrick M Vanderboom[2]; Angela Dispenzieri[2]; David L Murray[2]; Paul M Thomas[1]; Neil L Kelleher[1]; [1]*Northwestern University, Evanston, IL;* [2]*Mayo Clinic, Rochester, MN*

WP 223 **Isotopic Peak Index: A Novel Nomenclature to Help Simultaneously Detect and Identify 13 IGF-1 Variants during Routine Clinical Analysis**; Ievgen Motorykin[1]; Michael P Caulfield[1]; Michael J McPhaul[1]; Zengru Wu[1]; [1]*Quest Diagnostics, San Juan Capistrano, CA*

WP 224 **Case-Control Study: Expanded Proteomics and Lipidomic Profiling for Early Prediction of Major Adverse Cardiac Events**; Qin Fu[1]; Irina Tchernyshyov[1]; Ronald Holewinski[1]; Vidya Venkatraman[1]; David Sarracino[2]; Casey Johnson[1]; Kelly Njine Mouapi[1]; Susan Cheng[3]; Chrisandra Shufelt[3]; Brennan Spiegel[4]; Noel Bairey Merz[3]; Scott Peterman[2]; Jennifer Van Eyk[1,3]; [1]*Advanced Clinical Biosystems Research Institute, The Smidt Heart Institute, Cedars-Sinai Medical Center, Los Angeles, CA 90048, Los Angeles,, CA;* [2]*Thermo Fisher Scientific, Cambridge, MA;* [3]*Barbra Streisand Women's Heart Center, The Smidt Heart Institute, Cedars-Sinai Medical Center, Los Angeles, CA;* [4]*Clinical and Translational Science Institute, Cedars-Sinai Medical Center, Los Angeles, CA*

WP 225 **Biomarker Detection Utilizing a Desktop IMS-MS Device with Electrospray Ionization High Resolution Drift Time Ion Mobility-Linear Ion Trap Mass Spectrometer**; Julia L. Kaszycki[1]; Gregory F. Brabeck[1]; Aurelio La Rotta[1]; Ching Wu[1]; [1]*Excellims Corporation, Acton, MA*

WP 226 **The MasSpec Pen for the Rapid Detection of Primary Breast Cancer and Breast Cancer Metastasis**; Kyana Y Garza[1]; Jialing Zhang[1]; John Lin[1]; Stacey Carter[2]; James Suliburk[2]; Chandandeep Nagi[2]; Livia S Eberlin[1]; [1]*University of Texas at Austin, Department of Chemistry, Austin, TX;* [2]*Baylor College of Medicine, Houston, TX*

WP 227 **Ambient Mass Spectrometry Mapping of Lipid Fingerprints in Healthy and Cancerous Human Colorectal Tissues**; Yasmin Shanneik[1]; Emrys A. Jones[2]; Bipasha Chakrabarty[3]; Kaye J. Williams[4]; Omer Aziz[3]; Steven Pringle[2]; Adam W. McMahon[1]; [1]*Wolfson molecular imaging centre, The University of manchester, Manchester, United Kingdom;* [2]*Waters Corporation, Manchester, United Kingdom;* [3]*The Christie NHS Foundation Trust, Manchester, United Kingdom;* [4]*The University of Manchester, Division of Pharmacy & Optometry, Manchester, United Kingdom*

WP 228 **Quantitative N-Glycan Profiling of Clinical Tissue Samples by On-Line Fluorescence-MS Using a Rapid Labeling Tag**; Sarah Totten[1]; Andres Guerrero[2]; John Yan[3]; Aled Jones[3]; James D. Brooks[4]; Abel Bermudez[1]; Sharon J. Pitteri[1]; [1]*Stanford University School of Medicine, Canary Center at Stanford for Cancer Early Detection, Palo Alto, CA;* [2]*ProZyme, A part of Agilent, Hayward, CA;* [3]*ProZyme, Hayward, CA;* [4]*Department of Urology, Stanford University School of Medicine, Stanford, California*

WP 229 **Development of LC-MS/MS Method for Detection Endogenous Steroids**; Konrad Piotr Kowalski[1]; Joanna Waś[2]; Magdalena Niedolistek[2]; [1]*Masdiag Sp. z o.o., Warszawa, Poland;* [2]*Department of Medical Biology, Institute of Cardiology, Warsaw, Poland*

WP 230 **Structures for Lossless Ion Manipulations (SLIM)-Mass Spectrometry (MS) for High Resolution Ion Mobility Analysis of Immunosuppressive Drugs**; Kelly Wormwood[1]; Laura Maxon[1]; Daniel DeBord[1]; [1]*MOBILion Systems Inc., Exton, PA*

WP 231 **Method Development and Validation of LC-MS/MS Based Assay for Detection of Carfentanil and Norcarfentanil in Human Urine**; Difei Sun[1]; Danijela Konforte[1]; Jan Palaty[2]; [1]*Lifelabs Medical Laboratories, Toronto, ON;* [2]*Lifelabs Medical Laboratories, Burnaby, BC*

WP 232 **HarmCheck: Direct Mass Spectrometry Harm Reduction Drug Checking for use in the Opioid Overdose Crisis**; Scott A. Borden[1,2]; Jan Palaty[3]; Erik T. Krogh[1,2]; Christopher G. Gill[1,2,4,5]; [1]*Appl. Env. Res. Labs. (AERL), Vancouver Island University, Chemistry Department, Nanaimo, BC;* [2]*University of Victoria, Chemistry Department, Victoria, BC;* [3]*Lifelabs Medical Laboratories, Burnaby, BC;* [4]*Simon Fraser University, Chemistry Department, Burnaby, BC;* [5]*University of Washington, DEOHS, Seattle, WA*

WP 233 **Quantitative Proteomic Assessment of Differences and Stability of Human Serum and Plasma Proteins**; Sumio Ohtsuki[1]; Madoka Nanbu[1]; Shin Nishiumi[2]; Takashi Kobayashi[2]; Shingo Ito[1]; Takeshi Masuda[1]; Masaru Yoshida[2]; [1]*Kumamoto University, Kumamoto, Japan;* [2]*Kobe University, Kobe, Japan*

WP 234 **Probe ElectroSpray Ionization Mass Spectrometry for Cholangiocarcinoma Tumor and Healthy Tissues Rapid Identification**; Silvia Giordano[1]; Hidekazu Saiki[2]; Hiroki Nakajima[2]; Matteo Donadon[3]; Matteo Cimino[3]; Cristiana Soldani[3]; Barbara Franceschini[3]; Guido Torzilli[3]; Enrico Davoli[1]; [1]*Istituto di Ricerche Farmacologiche Mario Negri IRCCS, Milan, Italy;* [2]*Shimadzu Corporation, Kyoto, Japan;* [3]*Humanitas Clinical and Research Center IRCCS, Rozzano, Italy*

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WP 235 **Label-Free Drug Discovery with Mass Spectrometry: High-Throughput Screening of Enzyme Modulators as Anticancer Candidates**; Alireza Abdolvahabi[1]; John J. Bowling[1]; Duane G. Currier[1]; Zoran Rankovic[1]; [1]*St Jude Children's Research Hospital, Memphis, TN*

WP 236 **Drug Discovery Applications of ADE-OPP-MS (Acoustic-Droplet-Ejection coupled Open-Port-Probe Mass Spectrometry) Platform**; Hui Zhang[1]; Wenyi Hua[1]; Chang Liu[2]; Jianua Liu[1]; David Cox[2]; Anthony Carlo[1]; Matt Troutman[1]; Tom Covey[2]; [1]*Pfizer Inc., Groton, CT;* [2]*SCIEX, Concord, ON*

WP 237 **Acoustic Droplet Ejection (ADE) and Open Port Probe (OPP) Sampling Interface for High Throughput Analysis of ADME Assays**; Tom Hollenbeck[1]; John Isbell[1]; Patrick White[1]; Lucas Westling[1]; Ashley Chong[1]; Stefan Thibodeaux[2]; [1]*GNF (Novartis), San Diego, CA;* [2]*Novartis, Cambridge, MA*

WP 238 **High-Throughput Analysis of Synthetic Samples from High-Density Microplates with ESI-MS Enabled by the Acoustic-Droplet-Ejection to the Open-Port Probe sampling interface**; Wenyi Hua[1]; Chang Liu[2]; Kenneth Dirico[1]; Joseph Tucker[1]; Thomas R. Covey[2]; Hui Zhang[1]; *[1]Pfizer Inc., Groton, CT; [2]SCIEX, Concord, ON*

WP 239 **Effect of Increased Plate Density on Sensitivity in High-Throughput LDTD-MS**; Pierre Picard[1]; Pier-Luc Plante[2]; Sarah Demers[1]; Serge Auger[1]; Jean Lacoursière[1]; *[1]Phytronix Technologies, Inc., Quebec, QC; [2]Université Laval, Quebec, Quebec*

WP 240 **Enzyme Activity Assay of an Engineered Human Homocyst(e)inase in Mammalian Serum using LC-MS/MS**; Dale Schoener[1]; Silvia Ferrati[2]; Forrest Helfrich[1]; Jennifer Zarzoso[1]; Susan Alters[2]; Mike Buonarati[1]; *[1]Intertek Pharmaceutical Services, San Diego, CA; [2]Aeglea Biotherapeutics, Austin, TX*

WP 241 **Improved Kinome Coverage and Automated Data Analysis Pipeline for Large-Scale Kinase Inhibitor Screens**; Maria Reinecke[1,2]; Florian Seefried[1]; Svenja Petzold[1,2]; Tobias Schmidt[1]; Patroklos Samaras[1]; Mathias Wilhelm[1]; Stephanie Heinzlmeir[1]; Benjamin Ruprecht[1]; Guillaume Medard[1]; Bernhard Kuster[1]; *[1]Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; [2]German Cancer Consortium (DKTK), DKFZ partner site, Munich, Germany*

WP 242 **MS-Based Drug-Screening Platform for *in vitro* Biomedical Efficiency and *in vivo* Target Engagement of Covalent Inhibitors against KRAS G12C Mutant**; Shujia Dai[1]; Junqing Shen[1]; Gejing Deng[1]; Hong Cheng[1]; Bailin Zhang[1]; *[1]Biochemistry & Bioanalytics, Translational Sciences, Sanofi US, Cambridge, MA*

WP 243 **Characterization of a Novel BCL6 PROTAC to Provide Molecular Insights by Chemical Biology Approaches**; Fiona Pachl[1]; William McCoull[2]; Tony Cheung[3]; Kate Byth[3]; Aarti Kawatkar[1]; Timothy Rasmusson[1]; Paola Castaldi[1]; *[1]Discovery Sciences, IMED Biotech Unit, AstraZeneca, Waltham, MA; [2]Chemistry, IMED Biotech Unit, AstraZeneca, Cambridge, United Kingdom; [3]Bioscience, Oncology, IMED Biotech Unit, AstraZeneca, Waltham, MA*

WP 244 **Quantifying Heterogeneity in Drug-Uptake, Metabolism and Response in Single-Cells by an Integrated Raman-Spectroscopy and Mass spectrometry Approach**; Ahmed Ali[1]; Yasmine Abouleila[1]; Yoshihiro Shimizu[1]; Eiso Hiyama[2]; Arno Germond[1]; Toshio Yanagida[1]; *[1]RIKEN, Osaka, Japan; [2]Hiroshima University, Hiroshima, Japan*

WP 245 **High Resolution MS for 3D Culture Hepatic *in vitro* Models Metabolite Identification**; Sujoy Lahiri[1]; Kate Comstock[2]; *[1]Thermo Fisher Scientific, Frederick, MD; [2]Thermo Fisher Scientific, San Jose, CA*

WP 246 **Dual-Stream LC Coupled with 'Plug and Play' Automation for Routine Bioanalysis in Drug Discovery**; Emile G Plise[1]; Jonathan Cheong[1]; Katherine Gaffney[1]; Jamie Jorski[1]; Loren Olson[2]; Neal Liddle[2]; Anthony Romanelli[2]; Joseph Janiszewski[3]; Wayne Lootsma[3]; John Janiszewski[4]; *[1]Genentech, Inc., South San Francisco, CA; [2]SCIEX, Concord, ON; [3]Sound Analytics, Niantic, CT; [4]J2-Bioanalytical, Westerly, RI*

WP 247 **Development and Optimization of an Integrated Trap-and-Elute Microflow LC-MS/MS Platform**; Brendon Kapinos[1]; Mary Piotrowski[1]; Hui Zhang[1]; John Janiszewski[2]; Wayne Lootsma[3]; Steve Ainley[3]; *[1]Pfizer, Groton, CT; [2]J2-Bioanalytical, Westerly, RI; [3]Sound Analytics, Niantic, CT*

WP 248 **Stereoisomer Separation of Drugs and Biomarkers Using Supercritical Fluid Chromatography to Support PK/PD Studies**; Fangbiao Li[1]; Bang-lin Wan[2]; Guangping Bi[2]; Rena Zhang[2]; Daniel Spellman[2]; *[1]Merck & Co., Inc.,, West Point, PA; [2]Merck & Co., Inc., West Point, PA*

WP 249 **LC-MS for Bioanalysis of a Wide Range of Biotherapeutic Modalities**; Hao Jiang[1]; Alex Kozhich[1]; Linlin Luo[1]; Wendy Miller[1]; Craig Titsch[1]; Johanna Mora[1]; Gerry Kolaitis[1]; *[1]Bristol-Myers Squibb, Princeton, NJ*

WP 250 **Ion Mobility-Enabled Metabolite Identification of Tienilic Acid and Tienilic Acid Isomer**; Lauren Mullin[1]; Giorgis Isaac[1]; Ian D Wilson[2]; Gordon Murray[3]; Nathan Andersen[1]; Robert S Plumb[1]; *[1]Waters Corporation, Milford, MA; [2]Imperial College London, London, SW7 2AZ; [3]Waters Corp., Beverly, MA*

WP 251 **Structures for Lossless Ion Manipulations (SLIM)-Mass Spectrometry (MS) for High Resolution and High Throughput Glycan Biomarker Analysis**; Kelly Wormwood[1]; Liulin Deng[1]; Daniel DeBord[1]; Laura Maxon[1]; Hirsh Nanda[2]; Jarrat Jordan[2]; Sunil Nagpal[2]; Harsha Gunawardena[2]; *[1]MOBILion Systems Inc., Exton, PA; [2]Janssen Research and Development, Spring House, PA*

WP 252 **Pharmacokinetic Analysis of an Alzheimer's Disease Therapeutic in Rat Serum via 908devices ZipChip CZE-MS**; Zachary Kelley[1]; Mark Lovell[1,2]; Bert C. Lynn[1]; *[1]Department of Chemistry, University of Kentucky, Lexington, KY; [2]Sanders-Brown Center on Aging, University of Kentucky, Lexington, KY*

WP 253 **Streamlining the Metabolite Identification Workflow in Drug Discovery: Evaluation of Different Fragmentation Techniques and Software for Data Analysis**; Catalina Suarez[1]; Qi Wu[1]; Yongying Jiang[1]; *[1]MD Anderson Cancer Center, Houston, TX*

WP 254 **Evaluation of Microflow LC-MS/MS in a Quantitative Discovery Bioanalysis Setting**; Jun Zhang[1]; Wilson Shou[1]; Jonathan Ho[2]; Tairo Ogura[2]; Yohei Arao[2]; Shu Li[1]; Harold Weller[1]; *[1]Bristol-Myers Squibb, Hopewell, NJ; [2]Shimadzu Scientific Instruments, Inc., Columbia, MD*

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WP 255 **Development of a Multiple-Reaction Monitoring (MRM) LC-MS/MS Method for Detection of Microbial Transglutaminase from Streptomyces**; Rebekah L Sayers[1]; Jianru Stahl-Zeng[2]; *[1]SCIEX, Warrington, United Kingdom; [2]SCIEX, Darmstadt, Germany*

WP 256 **Application of REIMS to Describe Genetic, Environmental, and Processing Factors Affecting**; Harmonie M Bettenhausen; *Colorado State University, Fort Collins, CO*

WP 257 **Classification and Visualization of Beer Quality Using GC-MS and GC-FID**; Yusuke Takemori[1]; Yui Higashi[1]; Takero Sakai[2]; Ryo Takechi[3]; Motoki Sasaki[4]; Narihiro Suzuki[4]; *[1]Shimadzu Corpration, Kyoto, Japan; [2]Shimadzu Corporation, Nakagyo-ku, Japan; [3]Shimadzu Scientific Instruments, Inc., Columbia, Maryland; [4]Ise Kadoya Brewery, Ise, Japan*

WP 258 **MALDI-MS Analysis of Phospholipids from Colombian Cacao Beans**; Deisy Giraldo Davila[1]; Marianny Y. Combariza[1]; Cristian Blanco-Tirado[1]; *[1]Universidad Industrial de Santander, Bucaramanga, Colombia*

WP 259 **Non-Targeted Metabolomic Study on Variation of Phenolics in Different Cranberry Cultivars Using UPLC-IM-HRMS**; Yifei Wang[1,2]; Nicholi Vorsa[3]; Peter de B. Harrington[2]; Pei Chen[1]; *[1]U.S. Department of Agriculture, Agricultural Research Service, Beltsville Human Nutrition Research Center, Food Composition and Methods Development Laboratory, Beltsville, MD; [2]Center for Intelligent Chemical Instrumentation, Department of Chemistry & Biochemistry, Ohio University, Athens, OH; [3]Philip E. Marucci Center for Blueberry and Cranberry Research and Extension, Rutgers University, Chatsworth, NJ*

WP 260 **Comparing Chemical Constituency using Data-Driven Botanical Extraction Solvent Assessment by UHPLC-PDA-CAD-HRMS**; Christopher J. Pulliam[1]; Vincent P.

Sica[1]; Timothy R. Baker[1]; [1]*The Procter and Gamble Co., Cincinnati, OH*

WP 261 **Application of Metabolomics Methods on LC/GQ-QTOF Data to Discriminate Extra Virgin Olive Oils from Different Protected Designations of Origin;** Lucía Olmo-García[1]; Karin Wendt[2]; Nikolas Kessler[2]; Aadil Bajoub[3]; Artem Filipenko[4]; Alberto Fernández-Gutiérrez[1]; Carsten Baessmann[2]; Alegría Carrasco-Pancorbo[1]; [1]*Department of Analytical Chemistry, Faculty of Science, University of Granada, Granada, Spain;* [2]*Bruker Daltonik GmbH, Bremen, Germany;* [3]*Department of Basic Sciences, National School of Agriculture, Meknès, Morocco;* [4]*Bruker Daltonics Inc., Billerica, MA*

WP 262 **Phytochemicals and Their Metabolites as the Exposure Biomarkers of Whole Grain Intake;** Shengmin Sang[1]; Yingdong Zhu[1]; Pei Wang[1]; Shuwei Zhang[1]; Yao Tang[1]; [1]*North Carolina A&T State University, Kannapolis, NC*

WP 263 **Rapid-Throughput Characterization of Dietary Fiber Supplements Employing UHPLC/QqQ MS;** Thai-Thanh T Vo[1]; Matthew J. Amicucci[2]; Eshani Nandita[2]; Ace G. Galermo[1]; Megan A. Lee[2]; Yiyun Liu[2]; Carlito B. Lebrilla[2]; [1]*University of California Davis, Davis, CA;* [2]*University of California, Davis, Davis, CA*

WP 264 **The Effects of Boiling Time on the Wort Proteome during Beer Production;** Katherine Cordova[1]; Ray Bacala[1]; Marta Izydorczyk[1]; Dave Hatcher[1]; [1]*Canadian Grain Commission, Winnipeg, MB*

WP 265 **Lipid Profiling of Beef Muscle Tissues by LC-MS/MS and GC Analysis and Possible Health Benefits of Odd Chain Fatty Acids;** Beate Fuchs[1]; Dirk Dannenberger[1]; [1]*Leibniz-Institut für Nutztierbiologie (FBN), Dummerstorf, Germany*

WP 266 **Food Classification and Authenticity Testing Using a New High-Resolution LC/QTOF and Novel Classification Software;** Daniel Cuthbertson[1]; Karen E Yannell[2]; Frank Kuhlmann[2]; [1]*Agilent Technologies, Seattle, WA;* [2]*Agilent Technologies, Inc., Santa Clara, CA*

WP 267 **Effects of Purple Potato Rich Diet on Fecal Metabolome Profiles of Mice as Determined by Untargeted LC-MS/MS Screening;** Lili Mats[1]; Honghui Zhu[1]; Hua Zhang[1]; Rong Cao (Tsao)[1]; [1]*Agriculture and Agrifood Canada, Guelph, ON*

WP 268 **Metabolite Fingerprinting and Mapping the Phytonutrients through LCMS and HPTLC Analysis of Rice Varietals, Endogenous to North-East Region of India;** Krishna N Dutta[1]; Akanksha Singh[2]; Paramita Choudhury[1]; Rajlakshmi Devi[1]; Narayan C Talukdar[1]; Suman K Samanta[1]; Dipankar Malakar[2]; Manoj G Pillai[2]; [1]*Life Sciences Division, Institute of Advanced Study in Science and Technology, Guwahati, India;* [2]*SCIEX, Gurgaon, India*

WP 269 **The Selection of Tree Nut Peptide Markers: A Need for Improved Protein Sequences Databases;** Weili Xiong[1]; Melinda A. McFarland[1]; Cary Pirone[1]; Christine H. Parker[1]; [1]*FDA, College Park, MD*

WP 270 **Simple, Rapid, Dilute-and-Shoot Analysis of Triacylglycerols in Bovine Milk;** Michael Bukowski[1]; Matthew J. Picklo[1]; [1]*USDA/ARS, Grand Forks, ND*

WP 271 **Determination of Endocrine Disrupting Compounds in Lavender and Tea Tree Oils by MIP-SPE and HPLC-HRMS;** Paulina K Piotrowski[1]; Benjamin Place[1]; [1]*NIST, Gaithersburg, MD*

WP 272 **Contributing Factors of Fermentation Methods on Volatile Organic Compounds in Cider by Headspace Solid Phase Microextraction-GC-MS Analysis;** Matthew Bingman[1]; Jordanne Pelkey[1]; Claire Stellick[1]; Jared Scott[2,3]; Callie Cole[1]; [1]*Fort Lewis College, Durango, CO;* [2]*Pome LLC, Hesperus, CO;* [3]*Fenceline Cidery, Mancos, CO*

WP 273 **Evaluation of Trimethylamine in the De-Dimerization of 2-Hydroxy-4-(methylthio)butanoic Acid (HMB) Utilizing GC-MS and TMS- and tBDMS-Derivatization;** Thomas P Mawhinney[1]; Yiyi Li[1]; Deborah L Chance[1]; James K Waters[1]; [1]*University of Missouri, Columbia, MO*

WP 274 **In-Depth Profiling of Beetroot Bioactive Compounds by DAD-ESI-LC/MS/MS;** Nebiyu Abshiru[1]; Boris Nemzer[1]; [1]*VDF FutureCeuticals, Inc, Momence, IL*

WP 275 **Dereplication of Betalain Derivatives in Different Color of Djulis (Chenopodium formosanum) using UHPLC-DAD-ESI-Orbitrap;** Gui-ru Xie[1]; Hong-Jhang Chen[1]; [1]*National Taiwan University, Taipei, Taiwan*

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WP 276 **Veterinary Drug Detection in Pork and Milk Using a Small, Innovative Triple Quad with an ESI Ion Source;** Jarod Grossman[1]; Theresa Sosienski[1]; [1]*Agilent Technologies, Santa Clara, CA*

WP 277 **Determination of Acrylamide in Coffee by LC-MS/MS;** Jd De-Alwis[1]; Euan Ross[1]; Joanne Williams[1]; Kenneth Rosnack[2]; [1]*Waters, Wilmslow, United Kingdom;* [2]*Waters Corporation, Milford, MA*

WP 278 **Optimized System for Pulsed Injections and Backflushing in GC/MS Analysis of Pesticides with Acetonitrile Solvent;** Anastasia Andrianova[1]; Bruce Quimby[1]; [1]*Agilent Technologies, Wilmington, DE*

WP 279 **High-Throughput Online Miro-SPE with LCMS/MS Analysis of Multiple Pesticides Residues in Fruits and Vegetables;** jianzhong li[1]; Ye Kong[1]; Zhe Cao[1]; [1]*No.3,Wang Jing Bei Lu, Beijing, China*

WP 280 **Fast Analysis of Multi-Class Pesticides Panel in Wine and Olive Oil Extracts using a Single Run LC-Triple Quadrupole Mass Spectrometry;** Illaria Palini[1]; Silvia Bani[1]; Debora D'Addona[2]; Charles T. Yang[3]; Dipankar Ghosh[3]; [1]*ISVEA, Poggibonsi, Italy;* [2]*Thermo Fisher Scientific, Milano, Italy;* [3]*Thermo Fisher Scientific, San Jose, CA*

WP 281 **Determination of Glycoalkaloids in Potato by Molecular Imprinted Polymer@Magnetic Nanoparticles Combined with Liquid Chromatography Mass Spectrometry;** Cheng-Hsing Yeh[1]; Chung-Yu Chen[1]; Peipei Qi[2]; Maw-Rong Lee[1]; [1]*National Chung-Hsing University, Taichung, Taiwan;* [2]*Zhejiang Academy of Agricultural Sciences, Hangzhou, China*

WP 282 **Screening and Quantitation of Drugs Illegally Added to Health Foods by UHPLC-hybrid Quadrupole-Orbitrap Mass Spectrometry;** Long Sun[1]; Tao Bo[1]; [1]*Thermo Fisher Scientific, Beijing, China*

WP 283 **A Rapid and Original Method for the Determination of Heterocyclic Aromatic Amines in Cooked Meat using QuEChERS Extraction and UHPLC-APCI-MS/MS;** Sylvie Chevolleau[1,2]; Alyssa Bouville[1,2]; Laurent Debrauwer[1,2]; [1]*Axiom Platform, UMR 1331 Toxalim, MetaToul-MetaboHUB, National Infrastructure of Metabolomics and Fluxomics, Toulouse, France;* [2]*Toxalim, Université de Toulouse, INRA, INP-ENVT, INP-EI-Purpan, Université de Toulouse 3 Paul Sabatier, Toulouse, France*

WP 284 **Multi-class Veterinary Drug Screening and Quantitation with a Comprehensive Workflow;** Ed George[1]; Viet Dang[2]; [1]*ThermoFisher Scientific, San Jose, CA;* [2]*Iowa State University, Ames, IA*

WP 285 **Methodology for Detection and Structural Characterization of Phosphodiesterase-5 (PDE-5) Inhibitor Adulterants in an Herbal Coffee Product;** Marian Twohig[1]; Andy Aubin[1]; Sarah Dowd[2]; Gordon Fujimoto[2]; Simon Hird[3]; Kenneth Rosnack[1]; [1]*Waters Corporation, Milford, MA;* [2]*Waters Corporation, Beverly, MA;* [3]*Waters Corporation, Wilmslow, United Kingdom*

WP 286 **A Quantitative Method to Detect Penicillin in Limited Amounts of Bovine Tissues Using Liquid Chromatography and Tandem Mass Spectrometry (LC/MS/MS);** Linge Li[1]; Karyn D. Howard[1]; Christine Kilonzo[1];

Raoul Gonzales[1]; Michael Myers[1]; [1]*FDA/Center for Veterinary Medicine, Office of Research, Laurel, MD 20708*

WP 287 **Optimization of Detection and Separation Conditions in LC-MS/MS Method for Determination of Phenotiazine Dyes in Fish Muscle**; Luiza Kijewska[1]; Kamila Mitrowska[1]; Luigi Giannetti[2]; Bruno Neri[2]; [1]*Department of Pharmacology and Toxicology, National Veterinary Research Institute (PIWet), Pulawy, Poland;* [2]*Istituto Zooprofilattico Sperimentale Regioni Lazio e Toscana Via Appia Nuova, Rome, Italy*

WP 288 **Determination of Glyphosate in Animal Feed Matrices by QuPPe Extraction and LC-MS/MS Detection**; Joanne L Baillie[1]; Fang Shi[1]; [1]*Canadian Food Inspection Agency, Calgary, AB*

WP 289 **Sensitive Determination of Polar Anionic Pesticides in Wheat Flour by Stable Isotope Dilution Ion Chromatography–Tandem Mass Spectrometry**; Yingchen Li[1]; Qilei Guo[1]; Tao Bo[1]; [1]*Thermo Fisher Scientific, Beijing, China*

WP 290 **Fragmentation Pathways of Synthetic Drugs Added in Health Food Based on Higher Energy Collisional Dissociation in High-Resolution Quadrupole-Orbitrap Mass Spectrometry**; Long Sun[1]; Qilei Guo[1]; Tao Bo[1]; [1]*Thermo Fisher Scientific, Beijing, China*

WP 291 **QuEChERS Coupled to Gas Chromatography-Mass Spectrometry for Determination of Leachables of Packaging Material in Beverages**; Ya-Ying Chen[1]; Chung-Yu Chen[1]; Poppy Wulandari Sitanggang[1]; Peipei Qi[2]; Maw-Rong Lee[1]; [1]*National Chung-Hsing University, Taichung, Taiwan;* [2]*Zhejiang Academy of Agricultural Sciences, Hangzhou, China*

WP 292 **Combination of GC/MS/MS and LC/MS/MS to Analyze Multiclass Pesticides in Orange Using One QuEChERS Sample Preparation Method**; zhiming zhang[1]; Ge Meng[1]; Dan-hui Dorothy Yang[2]; Jianzhong Li[3]; Jinlan Sun[3]; Cuiling Wu[3]; [1]*Agilent Technologies (Shanghai) Co., Ltd., Shanghai, China;* [2]*Agilent Technologies, Santa Clara, CA;* [3]*Agilent Technologies(China) Co. Ltd., Beijing, China*

WP 293 **Analysis of Bifenazate and Derived Metabolite, Bifenazte-Diaen, in Six Livestock Products using Liquid Chromatography-Tandem Mass Spctrometry**; Da-Hee Park[1]; Kyung-Hee Yoo[1]; Seong-Kwan Kim[1]; Ho-Chul Shin[1]; [1]*Konkuk university, Seoul, South Korea*

WP 294 **Rapid and Easy Analysis of Tetrodotoxin by Direct Probe Ionization/Tandem Mass Spectrometry (DPiMS)**; Tasuku Murata[1]; Koretsugu Ogata[1]; Yuji Nagashima[2]; [1]*Shimadzu Corporation, Kyoto, Japan;* [2]*Food Industry, Department of Food Industry, Niigata Agro-Food University, Niigata, Japan*

WP 295 **Development of a Confirmatory Method for Determination of Xenobiotics in Honey by HPLC-MS/MS**; Pavel Metalnikov[1]; Ilya Batov[1]; Renat Selimov[1]; Denis Nekrasov[1]; Tatyana Sukhova[1]; Alexandre Komarov[1]; [1]*VGNKI, Moscow, Russian Federation*

WP 296 **Screening and Low-Level Quantitation of Chloramphenicol (CAP) in Commercial Honey Samples Using Miniaturized LC/MS System**; Vikrant Goel[1]; Saikat Banerjee[2]; Samir Vyas[3]; [1]*Agilent Technologies, Gurgaon, India;* [2]*Agilent Technologies India Pvt Ltd, Hyderbad, India;* [3]*Agilent Technologies India Pvt Ltd, Mumbai, India*

WP 297 **The Analysis of Chloramphenicol in Milk Using Ultra High Pressure Liquid Chromatography/Compact Mass Spectrometry**; Changtong Hao[1]; Daniel Eikel[1]; Simon Prosser[1]; [1]*Advion Inc., Ithaca, NY*

WP 298 **QuEChERS Extracted Pesticide Quantitation by LCMS QTOF using High Resolution Accurate Mass Acquisition Acquired at High Data Acquisition Speed**; Alan Barnes[1]; Steve Williams[2]; Christopher Titman[1]; Neil Loftus[1]; [1]*Shimadzu Corporation, Manchester, United Kingdom;* [2]*Concept Life Sciences, Cambridge, United Kingdom*

WP 299 **High-Throughput Analysis of Indole, Skatole and Androstenone in Pork Fat Using a LDTD-MS/MS System**; Jean Lacoursière[1]; Serge Auger[1]; Sarah Demers[1]; Pierre Picard[1]; [1]*Phytronix Technologies, Quebec, QC*

WP 300 **Thyreostatic Drug Analysis in Animal Tissues using LC-SRM and High-Field Asymmetric Waveform Ion Mobility Spectrometry (FAIMS)**; Randall W Purves[1, 2]; Kim Souster[1]; Caleb M.E. Fisher[1]; Michelle West[1]; Roger Munro[1]; Haixia Zhang[2]; Michael W. Belford[3]; Albert Vandenberg[2]; Bryn O Shurmer[1]; [1]*Canadian Food Inspection Agency, Saskatoon, SK;* [2]*University of Saskatchewan, Saskatoon, SK;* [3]*Thermo Fisher Scientific, San Jose, CA*

WP 301 **Off-Line Hydrogen Cleaning of GC/MS Ion Source Increases Sample Throughput for Pesticides in Foods**; Jochen Stoeppler[1]; Joerg Riener[2]; Klaus Wilmers[1]; Thorsten Bernsmann[1]; Courtney Milner[3]; [1]*Chemisches und Veterinäruntersuchungsamt Münsterland-Emscher-Lippe (CVUA-MEL), Muenster, Germany;* [2]*Agilent Technologies, Waldbronn, Germany;* [3]*Agilent, Santa Clara, CA*

WP 302 **Is Washing and/or Cooking of Vegetables Enough to Minimize the Risk of Population Exposure to Pesticide Residues?**; Joshua Ye[1]; Jingcun Wu[2]; Erasmus Cudjoe[2]; Feng Qin[2]; [1]*PerkinElmer Inc., Woodbridge, ON;* [2]*PerkinElmer, Inc.,, Woodbridge, ON*

WP 303 **Rapid Measurement of Agrochemicals by PaperSpray Mass Spectrometry**; Steven Lawrence Reeber[1]; Neloni R. Wijeratne[1]; Mary L. Blackburn[1]; [1]*Thermo Fisher Scientific, San Jose, CA*

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WP 304 **Reduction of Disulfide Bonds Using a High-Powered Femtosecond Laser**; Simon K. Gammelgaard[1, 2]; Steffen B. Petersen[2]; Kim F. Haselmann[1]; Peter Kresten Nielsen[1]; [1]*Novo Nordisk A/S, Måløv, Denmark;* [2]*Aalborg University, Aalborg, Denmark*

WP 305 **Impact of Charge Sites on Fragmentation of Peptides and Proteins: Carbamylation and Guanidination**; Amanda Helms[1]; Jennifer S Brodbelt[1]; [1]*University of Texas at Austin, Austin, TX*

WP 306 **GC-MS with Photoionization of Cold Molecules in Supersonic Molecular Beams – Approaching the Softest Ionization Method**; Alexander B. Fialkov[1]; Elias Ikonen[2]; Tiina Laaksonen[2]; Aviv Amirav[1]; [1]*Tel-Aviv University, Tel-Aviv, Israel;* [2]*Neste Oyj, Porvoo, Finland*

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WP 307 **New Evaluation Methods for Expanding an Electron Ionization Mass Spectral Library**; Weihua Ji[1]; Sanford P. Markey[1]; Gary Mallard[1]; Dmitrii V. Tchekhovskoi[1]; Yuri A. Mirokhin[1]; Oleg V. Toropov[1]; Alexey Mayorov[1]; William E. Wallace[1]; Stephen E. Stein[1]; [1]*NIST, Gaithersburg, MD*

WP 308 **Improved Separation and Identification of Essential Oil Constituents in Commercial Products using GCxGC-HR-ToF-MS**; Vimbai Mhuka[1]; Simiso Dube[2]; Mathew M Nindi[2]; [1]*UNISA, Florida Park, Roodepoort, South Africa;* [2]*UNISA, Florida Park, Roodepoort, South Africa*

WP 309 **Rapid "Shotgun" APGC-Ion Mobility Mass Spectrometry for the Analysis of Phytosterols in Honey Bee Dietary Pollen**; Jeffrey T Morre[1]; Priyadarshini Chakrabarti[1]; Diana Oppenheimer[1]; Ramesh R Sagili[1]; Claudia S. Maier[1]; [1]*Oregon State University, Corvallis, OR*

WP 310 **Is a Never-Clean Ion Source Possible? Is it Possible to Prove It?**; Lorne Fell[1]; Todd Richards[1]; Joseph E Binkley[1]; [1]*LECO Corporation, St Joseph, MI*

WP 311 **Comprehensive Evaluation of NIST Library Search Software**; Arun Moorthy[1]; Anthony J Kearsley[1]; William E. Wallace[1]; Stephen E. Stein[1]; [1]*NIST, Gaithersburg, MD*

WP 312 **Combining Deconvolution, Library Search, and Principal Component Analysis to Detect and Identify Important Flavour and Fragrance Compounds with High-Resolution GC/MS**; Jason Cole[1]; John Voss[1]; Xin Zheng[2]; Scott Quarmby[1]; *[1]Thermo Fisher Scientific, Ausitn, TX; [2]Thermo Fisher Scientific, Austin, TX*

WP 313 **Improving GC/MS Library Search on a Single Quadrupole Using Complementary and Orthogonal Metrics Within the Run**; Don Kuehl[1]; Stacey Simonoff[1]; Yongdong Wang[1]; *[1]Cerno Bioscience, Norwalk, CT*

WP 314 **Progress in the Development of a Plasma Based CI-Source for GC-MS**; Kai Kroll[1]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany*

WP 315 **What is Identification?: Comprehensive Characterization of Exposome Samples via GCxGC-High Resolution TOFM**; Todd Richards[1]; Joseph E Binkley[1]; David Alonso[1]; Lorne Fell[1]; *[1]LECO Corporation, St Joseph, MI*

WP 316 **Stir Bar Sorptive Extraction-in-port Derivatization-Gas Chromatography-Mass Spectrometry for Determination of Perfluorocarboxylic Acids in Environmental Water**; Chun-Hung Wang[1]; Chung-Yu Chen[1]; Maw-Rong Lee[1]; *[1]National Chung-Hsing University, Taichung, Taiwan*

WP 317 **Comprehensive Analysis of Short-Chained Chlorinated Paraffins and other POPs in Environmental Samples by GCxGC-HR-TOFMS with a Novel Ion Source**; Scott Pugh[1]; George Tikhonov[1]; Viatcheslav Artaev[1]; *[1]LECO Corporation, St Joseph, MI*

WP 318 **Determination of Methamphetamines in Human Saliva by GC-MS and Two Step Injection On-Column derivatization**; Xiaolei Shi; *Shimadzu (China) Co., Ltd., Shanghai Office, Shanghai, China*

WP 319 **Comparing the Results of Trace Chemical Analyses of ~200 Compounds Using GC-HRMS vs. APGC-QQQ Systems**; Daryl Smith[1]; Wendy Zhao[1]; Xiangjun Liao[1]; Sue Quade[1]; Amy Sadler[1]; Valerie Casey[1]; Thea Rawn[1]; *[1]Health Canada, Government of Canada, Ottawa, ON*

WP 320 **Emerging Contaminants in Valparaiso, Chile Rain Water: Changes in Composition and Concentration Levels over Fifteen Years (2003-2017)**; Olga Polyakova[1]; Viatcheslav Artaev[2]; Victor Vidal[3]; Francisco Cereceda[3]; Katalina Gonzalez Arincibia[3]; Albert Lebedev[1]; *[1]Moscow State University, Moscow, Russian Federation; [2]LECO Corporation, St Joseph, MI; [3]Universidad Técnica Federico Santa Maria, Valparaiso, Chile*

WP 321 **DMEITM Source with a Reaction Cell - A New Advances in Ion Generation for GC-MS/MS**; Harikrishnan Sukumar[1]; Heather Gamble[1]; Dante Sanchez[1]; Victor Titov[1]; Anna Komilova[1]; Reza Javahery[1]; *[1]PerkinElmer Inc., Woodbridge, ON*

WP 322 **Vacuum Assisted Sorbent Extraction (VASE) and a Dual-Column Thermal Desorption Approach for GC-MS Analysis of Trace-Level Polycyclic Aromatic Hydrocarbons**; Sage J. B. Dunham[1]; Victoria L. Node[1]; Daniel B. Cardin[1]; *[1]Entech Instruments Inc, Simi Valley, CA*

WP 323 **Vacuum Assisted Sorbent Extraction for the Detection of Butyric Acid and other Short-Chain Fatty Acids by Headspace-GCMS-Headspace without Derivatization**; Tyler B. Van Ry[1]; Sage J.B. Dunham[2]; Victoria L. Noad[2]; Daniel B. Cardin[2]; James Eric Cox[1]; *[1]Department of Biochemistry, University of Utah, Salt Lake City, UT; [2]Entech Insruments, Simi Valley, CA*

WP 324 **Detection and Quantification of Fragrance Allergens in Complex Matrices Using GC-Orbitrap MS Technology**; Richard Law[1]; Xin Zheng[2]; Cristian I Cojocariu[1]; Jason Cole[2]; *[1]Thermo Fisher Scientific, Runcorn, United Kingdom; [2]Thermo Fisher Scientific, Ausitn, TX*

WP 325 **Development of an Integrated Qualitative Analysis Coupled with EI and Soft Ionization Data for GC-HRTOFMS System**; Masaaki Ubukata[1]; Kenji Nagatomo[1]; Ayumi Kubo[1]; Takaya Satoh[1]; John Dane[2]; *[1]JEOL, Ltd., Tokyo, Japan; [2]JEOL USA, Inc., Peabody, MA*

WP 326 **Multicomponent Analysis of Metabolites in Chinese Caterpillar Fungus using Gas Chromatography-Triple Quadrupole Mass Spectrometry**; Xiaoming Bao[1]; Peng Tan[2]; Jun Fan[3]; Taohong Huang[3]; *[1]Shimadzu (China) Co., Ltd, Chengdu, China; [2]Chengdu Institute for Food and Drug Control, Chengdu, China; [3]Shimadzu (China) Co., Ltd, Shanghai, China*

WP 327 **Workflow Solutions for Direct Insertion, Real-Time Gas Chromatography -Mass Spectrometry**; Ken Lynam[1]; Angela Henry[1]; Luis Cuadra-Rodriguez[2]; Wei Song[1]; *[1]Agilent Technologies, Wilmington, DE; [2]Agilent Technologies, Santa Clara, CA*

WP 328 **A Novel Soft Ionization Plasma Source for GC-MS/MS Applications**; Mehrnaz Sarrafzadeh[1]; Charles Jolliffe[1]; Dmitry Valyaev[1]; Reza Javahery[1]; *[1]PerkinElmer Inc., Woodbridge, ON*

WP 329 **Dual Mode Ionization Source (DMEI Source)**; Anna Komilova[1]; Dante Sanchez[1]; Harikrishnan Sukumar[1]; Reza Javahery[1]; Harpreet Singh[1]; *[1]PerkinElmer, Inc.,, Woodbridge, ON*

GLYCOPROTEINS I
330-350

WP 330 **Comparison of the Ionization Efficiency of N-Linked Glycopeptides by Matrix Assisted Laser Desorption Ionization and Electrospray Ionization**; Richard J Bell[1]; Eric D Dodds[1]; *[1]University of Nebraska - Lincoln, Lincoln, NE*

WP 331 **Evaluating the Utility of a HILIC Model for Predicting Glycan Retention across Differing Stationary Phases and Tagging Chemistries**; Naglaa Sheiba[1]; Mark Han[2]; Ron Orlando[1]; *[1]Complex Carbohydrate Research Center, University of Georgia, athens, Georgia; [2]Reference Standards Laboratory, The United States Pharmacopeial Convention, Rockville, Maryland 20852*

WP 332 **Analysis of Mucin Proteins by Charge Detection Mass Spectrometry**; Lauren F Barnes[1]; Benjamin E Draper[1]; Nicholas A Lyktey[1]; Martin F Jarrold[1]; *[1]Indiana University, Bloomington, IN*

WP 333 **N-Linked Glycosylation Site Mapping in Prostate Cancer and Matched Normal Tissue: Defining Alterations in Glycan Microheterogeneity**; Sarah Michelle Totten[1]; Abel Bermudez[1]; Sharon J. Pitteri[1]; James D. Brooks[2]; *[1]Stanford University School of Medicine, Canary Center at Stanford for Cancer Early Detection, Palo Alto, CA; [2]Stanford University School of Medicine, Stanford, CA, 94305*

WP 334 **Analysis of O-glycosylated Biopharmaceuticals using an O-glycan dependent Endoprotease and LC-MS**; Andreas Nägeli[1]; Philip J. Widdowson[2]; Maria Nordgren[1]; Tom Buchanan[2]; Rolf Lood[1]; Fredrik Leo[1]; Helen Nyhlen[1]; Jonathan Sjögren[1]; Rowan Moore[2]; Fredrik Olsson[1]; *[1]Genovis AB, Lund, Sweden; [2]Thermo Fisher Scientific, Runcorn, United Kingdom*

WP 335 **Detection of Site-Specific N-Glycosylation on the AAV8 Capsid Protein using High-Resolution Mass Spectrometry**; Arya Aloor; *Georgia State University, Atlanta, GA*

WP 336 **Modification of Cell Membrane Glycosylation with Inhibitors and Characterization with nanoLC-MS**; Qing W Zhou[1]; Yixuan Xie[2]; Qiongyu Li[1]; Maurice Wong[3]; Carlito B Lebrilla[1]; *[1]University of California, Davis, Davis, CA; [2]Univerisity of California, Davis, Davis, CA; [3]University of California Davis, Davis, CA*

WP 337 **Ionic Charge Manipulation using Solution and gas-Phase Chemistry to Facilitate Analysis of Highly Heterogeneous Proteins by ESI-MS**; Yang Yang[1]; Chendi Niu[1]; Cedric E. Bobst[1]; Igor A. Kaltashov[1]; *[1]Department of Chemistry, University of Massachusetts-Amherst, 240 Thatcher Way, Life Science Laboratories N369, Amherst, MA*

WP 338 **Ion Mobility Collisional-Cross Section Values Facilitate Identification and Quantification of N-Glycan Structure Isomers and Permit Automated Processing of HILIC-UPLC-FLD-TIMS-CID-MS/MS data**; Sven Bahrke[1]; Robert Wilmanowski[1]; Sheira Mujica[2]; Wolfgang Jabs[2]; Stuart Pengelley[3]; Detlev Suckau[3]; *[1]Glycotope GmbH, Berlin, Germany; [2]Beuth-Hochschule, Berlin, Germany; [3]Bruker Daltonik GmbH, Bremen, Germany*

WP 339 **High Throughput Profiling of Glycans Released from Therapeutic Glycoproteins via micro-Permethylation at the CCRC**; Stephanie A Archer-Hartmann[1]; Asif Shajahan[1]; Nitin Tatyaso Supekar[1]; Christian Heiss[1]; Parstoo Azadi[1]; *[1]University of Georgia, Athens, GA*

WP 340 **Identification of N-Glycopeptides using Electron Transfer/High-energy Collision Dissociation (EThcD)**; Rui Zhang[1]; Xue Dong[2]; Jianhui Zhu[3]; David M. Lubman[3]; Yehia Mechref[2]; Haixu Tang[1]; *[1]Indiana University Bloomington, Bloomington, IN; [2]Texas Tech University, Lubbock, TX; [3]University of Michigan Medical Center, Ann Arbor, MI*

WP 341 **Analysis of IgA1 O-Glycosylation in Familial IgA Nephropathy**; Ellenore P. Craine[1]; Audra A. Hargett[2]; Hiroyuki Ueda[2, 3]; Yoshimi Ueda[2, 3]; Colin Reily[2]; Zina Moldoveanu[2]; Stacy D. Hall[2]; Dana V. Rizk[2]; Krzysztof Kiryluk[4]; Ali G. Gharavi[4]; Takashi Yokoo[3]; Bruce A. Julian[2]; Matthew Renfrow[2]; Jan Novak[2]; *[1]University of Alabama at Birmingham, Birmingham; [2]University of Alabama at Birmingham, Birmingham, Alabama; [3]The Jikei University School of Medicine, Tokyo, Japan; [4]Columbia University College of Physicians and Surgeons, New York, 10032*

WP 342 **Characterizing HIV-1 Envelope N-Glycan Shield: A Glycomics and Bioinformatics Method**; Audra Hargett[1]; Qing Wei[1]; Barbora Knoppova[2]; Stacy Hall[1]; Milan Raska[1, 2]; Zina Moldoveanu[1]; Todd Green[1]; Jan Novak[1]; Matthew B. Renfrow[1]; *[1]University of Alabama at Birmingham, Birmingham, AL; [2]Palacky University in Olomouc, Olomouc, Czech Republic*

WP 343 **Site Specific N-Glycosylation of Afamin Expressed in a Baculoviral System**; Mislav Novokmet[1]; Andreas Naschberger[2]; Stefan Lechner[2]; Bernhard Rupp[2]; Gordan Lauc[1, 3]; *[1]Genos, Glycoscience Laboratory, Borongajska cesta 83h, Croatia; [2]Department of Genetic Epidemiology, Medical University Innsbruck, Schöpfstr. 41, Austria; [3]University of Zagreb Faculty of Pharmacy and Biochemistry, A. Kovačića 1, Croatia*

WP 344 **Enzyme Toolkit for Selective Enrichment and Analysis of Mucin-Domain Glycoproteins**; Stacy Malaker[1]; Judy Shon[1]; Kayvon Pedram[1]; Nicholas M Riley[1]; Carolyn R Bertozzi[1, 2]; *[1]Stanford University, Palo Alto, CA; [2]Howard Hughes Medical Institute, Stanford, CA*

WP 345 **Improving the Glycomics Fidelity of Cancer Cells *in vitro* by using a Physiological Cell Culture Medium**; Junyao Wang[1]; Wenjing Peng[1]; Yehia Mechref[1]; *[1]Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas*

WP 346 **Glycopeptide Micro-Heterogeniety: A Case Study in Antibody Glycans**; Anand Patel[1]; Stefano Bonissone[1]; Natalie Castellana[1]; *[1]Digital Proteomics, LLC., San Diego, CA*

WP 347 **Identification of Core-Fucosylated Glycoprotein as Potential Biomarker of Alzheimer's Disease**; Ding Liu[1]; Cheng Ma[1]; Peng George Wang[2]; *[1]Georgia state university, Atlanta, GA; [2]Georgia State University, Atlanta, GA*

WP 348 **Determination of Human Immunoglobulin Glycoforms by timsTOF Pro Sequencing Analysis**; Kim Alving[1]; Anjali Alving[2]; Aharon Cohen[1]; Bing Wang[1]; *[1]Sanofi, Waltham, MA; [2]Bruker Scientific, Billerica, MA*

WP 349 **Fast Analysis of Glycans using LC-MS and Proteinase K Digestion**; Suping Zheng[1]; Jie Ding[1]; *[1]PPD, Inc., Middleton, WI*

WP 350 **Characterizing Intact N-linked Glycoproteins with 2-Dimensional HPLC-MS: A Machine Learning Pipeline for Mapping Glycoproteoforms in Multidimensional Space**; Jiana Duan[1]; Weiwei Rong[1]; Shengkun Dai[1]; Steven Matthew Patrie[1]; *[1]Northwestern University, Evanston, IL*

HOMELAND SECURITY
351-360

WP 351 **Metabolomics in Nonhuman Primate Models for Radiation Biodosimetry in Emergency Preparedness**; Evan Pannkuk[1]; Evagelia C Laiakis[1]; Kirandeep Gill[1]; Shreyans K Jain[1]; Khyati Y. Mehta[1]; Denise Nishita[2]; Kim Bujold[3]; James Bakke[2]; Janet Gahagen[2]; Simon Authier[3]; Polly Chang[2]; Albert J Fornace[1]; *[1]Georgetown University, Washington Dc, DC; [2]SRI International, Menlo Park, CA; [3]CiToxLAB North America, Laval, QC*

WP 352 **A Clinical Assay for Botulinum Neurotoxins through Mass Spectrometric Detection**; Kaitlin M Hoyt[1]; Suzanne R Kalb[1]; John R. Barr[1]; Carolina Luquez[1]; Janet K. Dykes[1]; *[1]Centers for Disease Control and Prevention, Chamblee, GA*

WP 353 **Detection and Analysis of Simulated Chemical Warfare Agents via Portable Mass Spectrometry**; Camila Anguiano Virgen[1]; James D. Fox[2]; Jaime L. Winfield[2]; Kenneth C. Wright[2]; Guido F. Verbeck[1]; *[1]University of North Texas, Denton, TX; [2]Inficon, East Syracuse, NY*

WP 354 **Validation of an LC-MS/MS Method to Detect Ricin Activity**; Kathryn R. Pigg[1]; Jakub Baudys[1]; Dongxia Wang[1]; Suzanne R. Kalb[1]; John R. Barr[1]; *[1]Centers for Disease Control and Prevention, Atlanta, Georgia*

WP 355 **Sensitive Detection of Active Ricin by MALDI-TOF Mass Spectrometry through an Improved RNA Substrate**; Dongxia Wang[1]; Jakub Baudys[2]; John R Barr[2]; Suzanne R Kalb[2]; *[1]Centers of Disease Control and Prevention (CDC), Atlanta, GA; [2]Centers for Disease Control and Prevention, Atlanta, Georgia 30341*

WP 356 **Detection and Identification of Model Peroxide Explosives Using Paper Spray Ionization Combined With Tandem Mass Spectrometry**; Madeleine Wood[1, 2]; Luke Metzler[2]; Theodore Corcovilos[3]; Michael Van Stipdonk[2]; *[1]Forensic Science and Law Program, Duquesne University, Pittsburgh, PA; [2]Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA; [3]Department of Physics, Duquesne University, Pittsburgh, PA*

WP 357 **Method Development for the Identification of Trichothecenes: Mass Spectral Library Matching and Determination of Unknown Mycotoxins**; Maria C. Prieto Conaway[1]; Mark Dreyer[1]; Todd H. Corzett[1]; Brian P. Mayer[1]; Audrey P. Williams[1]; *[1]Lawrence Livermore National Laboratory, Livermore, CA/94550*

WP 358 **Detection and Quantitative Analysis of Ricin by Tryptic Digestion and PRM MS Method**; Jakub Baudys[1]; Dongxia Wang[1]; John R. Barr[1]; Suzanne R. Kalb[1]; *[1]Centers for Disease Control and Prevention, Atlanta, Georgia*

WP 359 **Rapid Identification and Antibiotic Susceptibility Determination for Anthrax (Bacillus anthracis) using Lethal Factor Endopeptidase Activity Coupled with MALDI-MS**; Jon Rees[1]; Yulanda Williamson[1]; Anne E Boyer[1]; Maribel Gallegos-Candela[1]; Renato Lins[2]; John R Barr[1]; *[1]CDC, Atlanta, GA; [2]Batelle, Columbus, OH*

WP 360 **High-Throughput Screening of Explosive Residues Using a Robust Thermal Extraction Ionization Source (TEIS)**; Pierre Negri[1]; Neil Davenport[2]; Ashley Sage[2]; Peter Luke[3]; Carl Fletcher[3]; *[1]SCIEX, Redwood City, CA; [2]SCIEX, Warrington, United Kingdom; [3]Mass Spec Analytical, Bristol, United Kingdom*

IMAGING MS: DISEASE MARKERS I
361-379

WP 361 **Lipid Profiling of Carotid Atherosclerotic Plaque with Mass Spectrometry Imaging**; Mirjam Visscher[1]; Astrid M. Moerman[1]; Peter C. Burgers[1]; Heleen M.M. Van Beusekom[1]; Antonius F.W. Van der Steen[1]; Theo M. Luider[1]; Kim Van der Heiden[1]; Gijs Van Soest[1]; *[1]Erasmus MC, Rotterdam, Netherlands*

WP 362 **A Novel Strategy for Cancer Biomarker Discovery Powered by Lipids Profiling using Imaging MS together with UPLC-QTOF/QQQ Tandem MS**; Lei Wang[1]; Xu Ma[1]; Chunyan Lan[1, 2]; Hainan Li[3]; Linbo Cai[3]; Xiaofei Jia[4]; Huiqin Zhong[4]; *[1]National Center for Human Genetic Resources, National Research Institute for Health and Family Planning, Beijing, China; [2]Peking Union Medical College Graduate School, Beijing, China; [3]Guang Dong San Jiu Brain Hospital, Guangzhou, China; [4]Waters Technologies (Shanghai) Co, Ltd, Shanghai, China*

WP 363 **Integrating Ambient Ionization Mass Spectrometry with Machine Learning for Rapid Breast Cancer Diagnosis**; Hsin-Hsiang Chung[1]; Ying-Chen Huang[1]; Bo-Rong Chen[2]; Ming-Yang Wang[2]; Cheng-Chih Hsu[1]; *[1]Department of Chemistry, National Taiwan University, Taipei, Taiwan; [2]Department of Surgery, National Taiwan University Hospital, Taipei, Taiwan*

WP 364 **Discrimination of Human Renal Oncocytoma from Normal Kidney and Renal Cell Cancer Subtypes Using Ambient Ionization Mass Spectrometry Imaging**; Jialing Zhang[1]; Shirley Li[1]; Wendong Yu[2]; Livia S Eberlin[1]; *[1]University of Texas at Austin, Austin, TX; [2]Baylor College of Medicine, Houston, TX*

WP 365 **3D MALDI Imaging of Traumatic Brain Injury:Unveiling a Link to Parkinson's Disease**; Khalil Mallah[1]; Jusal Quanico[1]; Dennis Trede[2]; Firas Kobeissy[3]; Isabelle Fournier[1]; Michel Salzet[1]; *[1]PRISM Inserm U1192 - University of Lille, Villeneuve D'ascq Cedex, France; [2]Bruker Daltonik GmbH, Bremen, Germany; [3]epartment of Biochemistry and Molecular Genetics, Faculty of Medicine, American University of Beirut, Beirut, Lebanon*

WP 366 **Predicting Lymph Node Metastasis in Endometrial Cancer by Multi-Modal Mass Spectrometry Imaging**; Parul Mittal[1]; Mark R Condina[2]; Matthew T Briggs[3]; Alice Ly[4]; Janina Oetjen[4]; Gurjeet Kaur Chatar Singh[5]; Manuela Klingler-Hoffmann[3]; Peter Hoffmann[3]; *[1]Adelaide Proteomics Centre, The University of Adelaide, Adelaide, Australia; [2]Future Industries Institute, Adelaide, Australia; [3]Future Industries Institute, Adelaide, Australia; [4]Bruker Daltonik GmbH, Bremen, Germany; [5]Institute for Research in Molecular Medicine, Universiti Sains Malaysia, Minden,, Malaysia*

WP 367 **Unraveling Pathogenesis of Renal Amyloidosis with MALDI Imaging Mass Spectrometry and Shotgun Proteomics on paraffin Embedded Renal Biopsy Tissue Section**; Yume Mukasa[1]; Yuki Kuzuhara[1]; Megumi Terada[1]; Takashi Nirasawa[2]; Ryo Kajita[2]; Marion Rabant[3]; Jean-Paul Duong Van Huyen[4]; Hatsue Ishibashi-Ueda[5]; Nobuto Kakuda[1]; Masaya Ikegawa[1]; *[1]Doshisha university, Kyotanabe City, Japan; [2]Bruker Japan K. K., Yokohama, Japan; [3]Necker-Enfants malads Hospital, Paris, France; [4]Georges-Pambidou European Hospital, Anatomy-Pathology, Paris, France; [5]National Cerebral and Cardiovascular Center Research Institute, Suita, Japan*

WP 368 **Lipid Fingerprint Enables Identification of Human Inflammatory Bowel Disease Using Imaging Mass Spectrometry**; Simona Saliyo[1]; Tom K. Abban[1]; Lucia Martín-Saiz[2]; Albert Maimó-Barceló[3]; Juan Bestard-Escalas[3]; Daniel H. López[3]; Sam Khorrami[3, 4]; Marcelo García[3, 4]; Gwendolyn Barceló-Coblijn[3]; Matthew E. Openshaw[1]; José A. Fernández[2]; *[1]Shimadzu, Manchester, United Kingdom; [2]Dep. of Physical Chemistry, Fac. of Science and Technology, University of the Basque Country (UPV/EHU), Bario Sarriena, Spain; [3]Institut d'Investigació Sanitària Illes Balears (IdISBa), Palma, Spain; [4]Gastroenterology Unit, Hospital Universitari Son Espases, Palma, Spain*

WP 369 **Mass Spectrometric In-Depth Proteome Analysis of the Kidneys from Rat Model of Diabetic Nephropathy**; Yuki Kuzuhara[1]; Yume Mukasa[2]; Takashi Nirasawa[3]; Ryo Kajita[3]; Hatsue Ishibashi-Ueda[4]; Nobuto Kakuda[2]; Masaya Ikegawa[1, 2]; *[1]Graduate School, Major of Medical Life Systems, Doshisha University, Kyotanabe City, Japan; [2]Department of Medical Life Systems, Doshisha University, Kyotanabe City, Japan; [3]Bruker Japan K.K., Yokohama, Japan; [4]National Cerebral and Cardiovascular Center Research Institute, Suita, Japan*

WP 370 **MALDI-MSI Investigation of Lipid Alterations in Developing Rat Cerebellum Following Hypoxic/Ischemic Insult**; Dominique Figueroa[1]; Maureen A. Kane[2]; *[1]University of Maryland Balitmore, Baltimore, MD; [2]University of Maryland, Baltimore, Baltimore, MD*

WP 371 **Bisphenol S Exposure Induced the Proliferation of Human Breast Tumor by Disturbing Lipid Metabolism and Protein Profiling**; Chao Zhao[1]; Zongwei Cai*[1]; *[1]Hong Kong Baptist University, HK, China*

WP 372 **Laser Desorption Ionization from Silicon Nanopost Arrays for Mass Spectrometry Imaging of Neutral Lipids in Bacterially Infected Human Skin Tissue**; Jarod Fincher[1]; Derek Jones[2]; Andrew Korte[1]; Jacqueline Dyer[1]; Paola Parlanti[1]; Anastas Popratiloff[1]; Christine Brantner[1]; Nicholas Morris[3]; Russell Pirlo[4]; Victoria Shanmugam[2]; Akos Vertes[1]; *[1]The George Washington University, Washington, DC; [2]The George Washington University, School of Medicine and Health Sciences, Washington, DC; [3]UES, Inc., Dayton, OH; [4]United States Naval Research Laboratory, Washington, DC*

WP 373 **Reproducibility of MALDI Imaging Based Tissue Classifications - Results of a Multi-Center Study**; Soeren-Oliver Deininger[1]; Rita Casadonte[2]; Petra Wandernoth[2]; Kristina Schwamborn[3]; Christine Bollwein[3]; Christian Marsching[4]; Katharina Kriegsmann[5]; Carsten Hopf[4]; Wilko Weichert[3]; Jörg Kriegsmann[2]; Peter Schirmacher[6]; Mark Kriegsmann[6]; Alice Ly[1]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Proteopath, Trier, Germany; [3]Institute of Pathology, Technical University of Munich, Munich, Germany; [4]Center for Biomedical Mass Spectrometry and Optical Spectroscopy (CeMOS), Mannheim University of Applied Sciences, Mannheim, Germany; [5]Department of Hematology, Oncology and Rheumatology, University Hospital Heidelberg, Heidelberg, Germany; [6]Institute of Pathology, University Hospital Heidelberg, Heidelberg, Germany*

WP 374 **Metabolomic/Lipidomic DESI Imaging of Different Cell Cultures**; Hadeer Mattar[1]; Emrys A. Jones[2]; Emmanuelle Claude[2]; Clare mills[1]; *[1]Division of Infection, Immunity & Respiratory Medicine, Manchester Institute of Biotechnology. University of Manchester, Manchester, United Kingdom; [2]Waters Corporation, Wilmslow, United Kingdom*

WP 375 **Spatial Information of Metabolites Using Mass Spectrometry Imaging on Breast Needle Biopsy Using DEFFI-MS**; Vincen Wu[1]; Paolo Inglese[2]; Hui-Yu Ho[2]; Andreas Dannhorn[3]; Emine Kazanc[2]; Goncalo Correia[2]; James Mckenzie[2]; Stephanie Ling[3]; Evdoxia Karali[4]; Nikolaos Koundouros[4]; Hiromi Kudo[2]; Peter Kreuzaler[5]; Sami Shousha[2]; Ian Gilmore[6]; Mariia Yuneva[5]; Richard Goodwin[3]; Josephine Bunch[6]; George Poulogiannis[4]; Zoltan Takats[2]; *[1]Imperial College London, London, United Kingdom; [2]Imperial College, London, United Kingdom; [3]AstraZeneca, iMED, United Kingdom; [4]Institute of Cancer Research, London, United Kingdom; [5]Francis Crick Institute, London, United Kingdom; [6]National Physical Laboratory, London, United Kingdom*



WP 376 **Mapping Molecular Interactions in the *Clostridium difficile* Infected Gastrointestinal Tract Using Multimodal Imaging Mass Spectrometry**; Emma R Guiberson[1,2]; Aaron G Wexler[3]; William J. Perry[1,2]; Eric P. Skaar[3]; Richard M. Caprioli[1,2,4,5,6]; Jeffrey M. Spraggins[1,2,4]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Department of Chemistry, Vanderbilt University, Nashville, TN; [3]Department of Pathology, Microbiology and Immunology, Vanderbilt University School of Medicine, Nashville, TN; [4]Department of Biochemistry, Vanderbilt University, Nashville, TN; [5]Department of Medicine, Vanderbilt University, Nashville, TN; [6]Department of Pharmacology, Vanderbilt University, Nashville, TN*

WP 377 **Multiple Chemical and Enzymatic Approaches for Comprehensive N-Glycome Determinations of Prostate Cancer Tissues by MALDI-FTICR Imaging Mass Spectrometry**; Connor A West[1]; Fred David[1]; Laura Spruill[1]; Anand Mehta[1]; Richard R Drake[1]; *[1]Medical University of South Carolina, Charleston, SC*

WP 378 **Desorption Electrospray Ionization Mass Spectrometry Imaging of Brain Tissue from a Mouse Model of Smith-Lemli-Opitz Syndrome**; Amy Li[1]; Libin Xu[1]; *[1]University of Washington, Seattle, WA*

WP 379 **A Novel Strategy for the Pathological Study of Alzheimer's Disease Brain with MALDI Imaging Mass Spectrometry with Shotgun Proteomics**; Masaya Ikegawa[1]; Nobuto Kakuda[1]; Tomohiro Miyasaka[1]; Takashi Nirasawa[2]; Ryo Kajita[2]; Shigeo Murayama[3]; Yasuo Ihara[4]; *[1]Doshisha university, Kyotanabe City, Japan; [2]Bruker Japan K.K., Yokohama, Japan; [3]The Brain Bank for Aging Research, Tokyo Metropolitan Geriatric Hospital and Institute of Gerontology, Tokyo, Japan; [4]Graduate School of Brain Science, Doshisha University, Kyotanabe City, Japan*

INFORMATICS: ALGORITHMS AND STATISTICAL ADVANCES II
380-402

WP 380 **A Ground Truth MS1 Data Set for Quantitative Evaluation of Precursor-Aware Proteomics Mass Spectrometry Data Processing Algorithms**; Jessica Henning[1]; Annika Tostengard[1]; Robert Smith[1]; *[1]University of Montana, Missoula, MT*

WP 381 **EnvCNN: A Convolutional Neural Network Model for Evaluating Isotopomer Envelopes in Top-Down Mass Spectral Deconvolution**; Abdul Rehman Basharat[1]; Zhe Wang[2]; Si Wu[2]; Rachele Lubeckyj[3]; Liangliang Sun[3]; Xiaowen Liu[1,4]; *[1]Department of BioHealth Informatics, Indiana University-Purdue University Indianapolis, Indianapolis, Indiana; [2]Department of Chemistry and Biochemistry, University of Oklahoma, Norman, Oklahoma; [3]Department of Chemistry, Michigan State University, East Lansing, Michigan; [4]Center for Computational Biology and Bioinformatics, Indiana University School of Medicine, Indianapolis, Indiana*

WP 382 **Targeted Database Search Strategies for Ricin Detection: Searching Only for Ricin Peptides**; Andy Lin[1]; Deanna Plubell[1]; Uri Keich[2]; William Stafford Noble[1]; *[1]University of Washington, Seattle, WA; [2]University of Sydney, Sydney, Australia*

WP 383 **MIND: A Double-Linear Model to Accurately Determine Monoisotopic Precursor Mass in High-Resolution Top-Down Proteomics**; Frederik Lermyte[1]; Piotr Dittwald[2]; Jürgen Claesen[3]; Geert Baggerman[4]; Frank Sobott[5]; Peter B. O'Connor[1]; Kris Laukens[4]; Jef Hooyberghs[6]; Anna Gambin[2]; Dirk Valkenborg[3]; *[1]University of Warwick, Coventry, United Kingdom; [2]University of Warsaw, Warsaw, Poland; [3]Hasselt University, Hasselt, Belgium; [4]University Of Antwerp, Antwerp, Belgium; [5]University of Leeds, Leeds, United Kingdom; [6]Flemish Institute for Technological Research (VITO), Mol, Belgium*

WP 384 **pValid: Validation Beyond the Target-Decoy Approach for Peptide Identification in Shotgun Proteomics**; Wen-Jing Zhou[1]; Hao Yang[1]; Wen-Feng Zeng[1]; Kun Zhang[1]; Hao Chi[1]; Si-Min He[1]; *[1]Institute of Computing Technology, CAS, Beijing, China*

WP 385 **Bayes' Formula and Fisher Information for Automated Analysis of Mass Spectra**; Alex Ulyanenkov[1]; Alexander Mikhalychev[2]; Svetlana Vlasenko[2]; *[1]Atomicus LLC, Seattle, WA; [2]Atomicus OOO, Minsk, Belarus*

WP 386 **MSstatsTMT: Statistical Detection of Differentially Abundant Proteins in Mass Spectrometry Experiments with Isobaric Labeling**; Ting Huang[1]; Meena Choi[1]; Manuel Tzouros[2]; Nikhil Janak Pandya[2]; Balazs Banfai[2]; Tom Dunkley[2]; Olga Vitek[1]; *[1]Northeastern University, Boston, MA 02115; [2]Roche Pharmaceutical Research and Early Development (pRED), Roche Innovation Center Munich, Germany*

WP 387 **Identification of Alternative-Splicing Events Present in Proteins Using Mass Spectrometry and a Custom Sequence Database of Junction-Spanned Peptides**; Bang-Jie Han[1]; Pang-Hung Hsu[1]; Wen-Shyong Tzou[1]; *[1]National Taiwan Ocean University, Keelung, Taiwan*

WP 388 **Tree Based Machine Learning Methods Improve Error Rates in Quality Control of Mass Spectrometry-Based Proteomics**; Eralp Dogu[1]; Shantam Gupta[2]; Roger Olivella[3]; Eduard Sabido[3]; Olga Vitek[4]; *[1]Mugla University, Mugla, Turkey; [2]Quantiphi Inc, Boston, Massachusetts; [3]CRG, Barcelona, Spain; [4]Northeastern University, Boston, MA*

WP 389 **Deep Learning Methods Applied to the Analysis of Metabolomics Data**; Shinji Kanazawa[1,2,3]; Yohei Yamada[1]; Hiroyuki Yasuda[1]; Akihiro Kunisawa[1]; Toru Shiohama[1]; Shigeki Kajihara[1]; Norio Mukai[1]; Masaki Kakisako[4]; Go Fujisawa[4]; Yuzuru Yamakage[4]; Junko Iida[1,2]; Eiichiro Fukusaki[5]; Fumio Matsuda[3]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Osaka University Shimadzu Analytical Innovation Research Laboratory, Osaka University, Osaka, Japan; [3]Graduate School of Information Science and Technology, Osaka University, Osaka, Japan; [4]Fujitsu Limited, Tokyo, Japan; [5]Graduate School of Engineering, Osaka University, Osaka, Japan*

WP 390 **SPIX, a Newly Developed Free Software to Overcome Operator Subjectivity in MS and Characterize Unknown Chemical Reactions in Complex Mixtures**; Edith Nicol[1]; Yao Xu[2,3]; Zsuzsanna Varga[1]; Stéphane Bouchonnet[1]; Marc Lavielle[2,3]; *[1]Laboratory of Molecular Chemistry, École Polytechnique, Palaiseau, France; [2]National Institute for Research in Computer Science and Automation (Inria), Saclay, France; [3]Center for Applied Mathematics, École polytechnique, Palaiseau, France*

WP 391 ***In vivo* Proteome Dynamics from Tandem Mass Spectrometry**; Ahmad Borzou[1]; Rovshan Sadygov[1]; *[1]University of Texas, Galveston, TX*

WP 392 **Diversity Indices Applied to Laser-Assisted Rapid Evaporative Ionisation MS (LA-REIMS) Microbial Profiles for Quality Control and Stratification for Classification Modelling**; Alvaro Perdones-Montero[1]; Simon Cameron[1]; Attila Kiss[2]; Richard Schaffer[2]; Julia Balog[2]; Keith Richardson[3]; Steven D Pringle[3]; Zoltan Takats[1]; *[1]Imperial College London, London, United Kingdom; [2]Waters Research Center Kft., Budapest, Hungary; [3]Waters Corporation, Wilmslow, United Kingdom*

WP 393 **The Titin Problem: Hitchhiking Siblings during Protein Inference**; Kyle Lucke[1]; Max Thibeau[1]; Levi Zell[1]; Julianus Pfeuffer[2]; Xiao Liang[3]; Oliver Serang[1]; *[1]University of Montana, Missoula, MT; [2]Eberhard Karls University of Tübingen, Tübingen, Germany; [3]Freie Universität Berlin, Berlin, Germany*

WP 394 **Improving Resource Libraries for Data Independent Acquisition through iRT Residual Prediction using Deep Learning**; Timothy Man[1]; Jan Muntel[1]; Roland Bruderer[1]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland*

WP 395 **Influence of Library Selection for Proteomics Experiments on Statistical Error Rate Estimation**; Seth Just[1]; Caleb Emmons[1]; Jacob C Lippincott[1]; Susan Ludwigsen[1]; Susan T Weintraub[2]; Brian C Searle[1,3]; *[1]Proteome Software, Portland, OR; [2]University of Texas Health Science Center at San Antonio, San Antonio, TX; [3]Institute for Systems Biology, Seattle, WA*

WP 396 **Updates on Philosopher: a complete toolkit for both conventional and open search-based shotgun proteomics data analysis**; Felipe Da Veiga Leprevost[1]; Avinash K Shanmugam[1]; Dattatreya Mellacheruvu[1]; Hui-Yin Chang[1]; Dmitry M Avtonomov[1]; Andy T. Kong[1]; Alexey I. Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, MI*

WP 397 **Automating Component Detection of Small Molecules in Complex Mixtures using HRAM Q-TOF data**; Simon Ashton[1]; Kirsten Hobby[1]; Alan Barnes[1]; Neil Loftus[1]; *[1]Shimadzu Corporation, Manchester, United Kingdom*

WP 398 **Extending the Scope of Prosit: Accurate Fragment Ion Intensity and Retention Time Prediction for (Un) Modified (Non-)Tryptic Peptides**; Tobias Schmidt[1]; Michael Graber[1]; Daniel P Zolg[1]; Siegfried Gessulat[1]; Patroklos Samaras[1]; Johannes Zerweck[2]; Tobias Knaute[2]; Hans-Christian Ehrlich[3]; Stephan Aiche[3]; Bernard Delanghe[4]; Andreas Huhmer[5]; Karsten Schnatbaum[2]; Ulf Reimer[2]; Bernhard Kuster[1]; Mathias Wilhelm[1]; *[1]Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; [2]JPT Peptide Technologies GmbH, Berlin, Germany; [3]SAP SE, Potsdam, Germany; [4]Thermo Fisher Scientific, Bremen, Germany; [5]Thermo Fisher Scientific, San Jose, CA*

WP 399 **Reducing False Peptide-Spectrum Matches in Peptide Identification using Spectrum Clustering**; Lei Wang[1]; Sujun Li[1]; Haixu Tang[1]; *[1]Indiana University Bloomington, Bloomington, IN*

WP 400 **Computing Information Content of PTM Site Localization Assignments Using PTMProphet**; David D. Shteynberg[1]; Eric W. Deutsch[1]; David S. Campbell[1]; Michael R. Hoopmann[1]; Ulrike Kusebauch[1]; Zhi Sun[1]; Anthony Whetton[2]; Robert L. Moritz[1]; *[1]Institute for Systems Biology, Seattle, Washington; [2]University of Manchester, Manchester, United Kingdom*

WP 401 **IsoSpec 2.0: a Hyperfast Fine Isotopic Envelope Calculator**; Michał Startek[1]; Mateusz K. Łącki[2]; Dirk Valkenborg[3,4,5]; *[1]University of Warsaw, Warsaw, Poland; [2]University Medical Center Mainz, Mainz, Germany; [3]Centre for Proteomics (University of Antwerp/VITO (Belgium)), Antwerp, Belgium; [4]Flemish Institute for Technological Research (VITO), Mol, Belgium; [5]Interuniversity Institute for Biostatistics ans Statistical Bioinformatics, Hasselt, Belgium*

WP 402 **A Novel Data-Adaptive Robust Method for Quantifying Tissue Specificity Scores**; Meng Wang[1]; Lihua Jiang[2]; Hua Tang[2]; Michael Snyder[2]; *[1]Stanford University, Stanford; [2]Stanford University, Palo Alto, CA*

INFORMATICS: METABOLOMICS
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WP 403 **Revealing Concurrent Change of Heterogeneity and Subpopulations of Cancer Cells Using Single Cell Metabolomics**; Renmeng Liu[1]; Jiannong Li[2]; Ann Chen[2]; Zhibo Yang[1]; *[1]Department of Chemistry and Biochemistry, University of Oklahoma, Norman, Oklahoma; [2]Department of Biostatistics and Bioinformatics, H. Lee Moffitt Cancer Center and Research Institute, Tampa, Florida*

WP 404 **Incorporating In-Source Fragments Improves Metabolite Identification Accuracy in Untargeted LC–MS and LC–MS/MS Datasets**; Jacob C Lippincott[1]; Phillip M Seitzer[1]; Brian C Searle[1,2]; *[1]Proteome Software, Portland, OR; [2]Institute for Systems Biology, Seattle, WA*

WP 405 **Automated Protein Metabolite Structure Elucidation Using HPLC/ESI-Exact Mass-MSMS Data for Insulin and ANP**; Marshall M. Siegel[1]; Gary E Walker[1]; Ronnie Crepeau[1]; Serhiy Hnatyshyn[2]; Asoka Ranasinghe[2]; *[1]MS Mass Spec Consultants, Fair Lawn, NJ; [2]Bristol-Myers Squibb Co., Lawrenceville, NJ*

WP 406 **Metabolic Profiling of Small Molecule Ion Mobility Assisted Data Independent Acquisition Data Using Skyline**; Brian S Pratt[1]; Johannes PC Vissers[2]; Ian D Wilson[3]; Nyasha C Munjoma[2]; Marine PM Letertre[3]; Micheal J MacCoss[1]; Brendan X MacLean[1]; *[1]University of Washington, Seattle, WA; [2]Waters Corporation, Wilmslow, United Kingdom; [3]Section of Computational and Systems Medicine, Imperial College, London, United Kingdom*

WP 407 **Exploratory Data Analysis and Interactive Visualization of FTICR-MS Data**; Allison M. Thompson[1,2]; Lisa M. Bramer[1]; Amanda M. White[1]; Kelly G. Stratton[1]; Daniel Claborne[1]; Kirsten S. Hofmockel[1,2]; Lee Ann McCue[1,2]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA*

WP 408 **SIRIUS 4 - Turning Tandem Mass Spectra into Metabolite Structure Information**; Kai Dührkop[1]; Markus Fleischauer[1]; Marcus Ludwig[1]; Martin A. Hoffmann[1]; Juho Rousu[2]; Sebastian Böcker[1]; *[1]Friedrich-Schiller University, Jena, Germany; [2]Aalto University, Espoo, Finland*

WP 409 **A Novel Approach to Data-Driven Differential Network Analysis with Limited Sample Size In High-Throughput Metabolomics and Lipidomics Data**; Gayatri R Iyer[1]; Janis Wigginton[2]; William Duren[1,2]; Marci Brandenburg[1,3]; George Michailidis[2,4]; Alla Karnovsky[1]; *[1]Department of Computational Medicine and Bioinformatics, University of Michigan Medical School, Ann Arbor, MI; [2]Michigan Regional Comprehensive Metabolomics Resource Core, Ann Arbor, MI; [3]Taubman Health Sciences Library, University of Michigan Medical School, Ann Arbor, MI; [4]Department of Statistics, University of Florida, Gainsville, FL*

WP 410 **Web Based Basic Mass Spectrometry Search Tool For Molecules To Search Public Data**; Mingxun Wang[1]; Alan K. Jarmusch[1]; Ricardo R. da Silva[1]; Robert Quinn[2]; Alexey Melnik[1]; Julia M Gauglitz[1]; Justin van der Hooft[1]; Andrés Rodríguez[1]; Louis Felix Nothias[1]; Jeremy Carver[1]; Jeramie Watrous[1]; Mohit Jain[1]; Rob Knight[1]; Nuno Bandeira[1]; Pieter C. Dorrestein[1]; *[1]UCSD, La Jolla, CA; [2]Michigan State University, East Lansing*

WP 411 **A Novel Tool for Evaluation of Data Preprocessing – an Essential Step in Untargeted Metabolomics**; Yasin El Abiead[1,2,3]; Maximilian Milford[1]; Gunda Koellensperger[1,2,3]; *[1]University of Vienna, Department of Analytical Chemistry, Vienna, Austria; [2]Vienna Metabolomics Center (VIME), Vienna, Austria; [3]Chemistry Meets Microbiology, Vienna, Austria*

WP 412 **Evaluation of Freely Available Software Tools for Untargeted Quantification of 13C Isotopic Enrichment in Cellular Metabolome from HR-LCMS Data**; Manohar Dange[1]; Vivek Mishra[1]; Murtaza Saiffudin Merchant[1]; Damini Jaiswal[1]; Bratati Mukherjee[1]; Charulata B Prasannan[1]; Pramod P Wangikar[1]; *[1]Indian Institute of Technology Bombay, Mumbai, India*

WP 413 **Feature-Based Molecular Networking of Untargeted Mass Spectrometry Data: Bridging MS-DIAL, MZmine2, MetaboScape, OpenMS, and XC-MS, with the GNPS Web-Platform**; Louis Felix Nothias[1]; Daniel Petras[1]; Mingxun Wang[1]; Robin Schmid[1,2]; Abinesh Sarvepalli[1]; Zheng Zhang[1]; Ricardo da Silva[1]; Pieter Dorrestein[1]; *[1]University of California, San Diego, La Jolla, CA; [2]University of Muenster, Institute of Inorganic and Analytical Chemistry, Muenster, Germany*

WP 414 **Deuterater: An Analyte-Agnostic Refactoring of Kinetic Analysis Software for Deuterium-Labeled Metabolomics**; Kyle J Cutler[1]; Russell Denton[1]; John C Price[1]; *[1]Brigham Young University, Provo, UT*

WP 415 **Using Cloud Computing for Large Scale Data Processing in Clinical Metabolomics**; Oliver Fiehn[1]; Ying Zhang[1,2]; Brian C DeFelice[1]; Sili Fan[1]; Diego Pedrosa[1]; Sajjan S Mehta[1]; Gert Wohlgemuth[1]; *[1]UC Davis West Coast Metabolomics Center, Davis, CA; [2]Chemistry Department UC Davis, Davis, CA*

WP 416 **Using Maximum Common Substructures to Interpret Hit Lists from Small-Molecule Tandem Hybrid Similarity Searches**; Brian T. Cooper[1,2]; Arun S Moorthy[2]; Tytus D Mak[2]; Stephen E Stein[2]; *[1]UNC Charlotte, Charlotte, NC; [2]NIST, Gaithersburg, MD*

WP 417 **MetaboQuest: Tool for Metabolite Identification**; Mohammad R Nezami Ranjbar[1]; Linge Yan[1]; Yan Gao[1]; Habtom W Ressom[1]; *[1]OmicsCraft LLC, Washington, District of Columbia*

WP 418 **A High-Resolution Accurate-Mass GC Electron Ionization (EI) and Chemical Ionization (CI) mass Spectral Database of Chemical Standards**; Biswapriya Biswavas Misra[1]; Michael Olivier[1]; *[1]Wake Forest Baptist Medical Center, Winston-Salem, NC*

WP 419 **The Power of MS/MSALL Acquisition for High-Throughput Metabolomics Studies**; Mariateresa Maldini[1]; Eva Duchoslav[2]; Cyrus Papan[3]; Khatereh Motamedchaboki[4]; *[1]SCIEX, Milan, Italy; [2]SCIEX, Concord, ON; [3]SCIEX, Darmstadt, Germany; [4]Sciex, Redwood City, CA*

WP 420 **Evaluations Factors for Intra- and Inter-Batches Variations in Targeted and Untargeted Metabolomics through SPC and QC-Dependent SC Strategies**; Li Zhang[1,2]; Peter Sajjakulnukit[1]; Maureen Kachman[2]; Costas Lyssiotis[1]; *[1]University of Michigan Medical School, Cancer Center, Ann Arbor, Michigan; [2]University of Michigan Medical School, BRCF Metabolomics Core, Ann Arbor, Michigan*

WP 421 **MetGem Software for the Generation of Molecular Networks Based on the t-SNE Algorithm**; Nicolas Elie[1]; Florent Olivon[1]; Gwendal Grelier[1]; Fanny Roussi[1]; Marc Litaudon[1]; David Touboul[1]; *[1]CNRS-ICSN, Gif-Sur-Yvette, France*

WP 422 **Characterizing Product Ions in a Reference Tandem Mass Spectral Library**; Xiaoyu Yang[1]; Pedatsur Neta[1]; Yuri Mirokhin[1]; Dmitrii Tchekhovskoi[1]; Yuxue Liang[1]; Alexey Mayorov[1]; Stephen E. Stein[1]; *[1]NIST, Gaithersburg, MD*

WP 423 **Development of a Machine Learning Tool to Enhance Gas Chromatography-Mass Spectrometry-Based Metabolite Identification**; Feng Qiu[1,2,3,4]; Zhentian Lei[1,2,3,5]; Lloyd W. Sumner[1,2,3,5]; *[1]Department of Biochemistry, University of Missouri, Columbia, MO; [2]Bond Life Sciences Center, University of Missouri, Columbia, MO; [3]Interdisciplinary Plant Group, University of Missouri, Columbia, MO; [4]International Flavors & Fragrances, Union Beach, NJ; [5]Metabolomics Center, University of Missouri, Columbia, MO*

WP 424 **Secondary Chemical Processes of Acylcarnitines Revealed by LC-MS/MS**; Xinjian Yan[1]; Sanford P. Markey[1]; Yamil Simón-manso[1]; Ramesh Marupaka[1]; Qian Dong[1]; Stephen E. Stein[1]; *[1]NIST, Gaithersburg, MD*

WP 425 **Contextualizing Metabolomics Data by Integrating Text Mining and Computational Chemistry**; Magnus Palmblad; *Leiden University, Leiden, Netherlands*

WP 426 **Computational metabolomics to characterize metabolites in stable isotope-labeled organisms**; Hiroshi Tsugawa[1]; Ryo Nakabayashi[1]; Tetsuya Mori[1]; Yutaka Yamada[1]; Mikiko Takahashi[1]; Amit Rai[2]; Ryosuke Sugiyama[1]; Hiroyuki Yamamoto[3]; Taiki Nakaya[2]; Mami Yamazaki[2]; Rik Kooke[4]; Johanna A. Bac-Molenaar[4]; Nihal Oztolan-Erol[4]; Joost J.B. Keurentjes[4]; Masanori Arita[1]; Kazuki Saito[1]; *[1]RIKEN, Yokohama, Japan; [2]Chiba University, Chuo-ku, Japan; [3]Human Metabolome Technologies, Tsuruoka, Japan; [4]Wageningen University & Research, Netherlands*

WP 427 **Uniting Metabolomics Data Processing and Highly Confident Annotation across Six MS Instrumental Set Ups: MetaboScape 5.0**; Nikolas Kessler[1]; Wiebke Timm[1]; Sascha Winter[1]; Ulrike Schweiger-Hufnagel[1]; Sven W. Meyer[1]; Aiko Barsch[1]; Heiko Neuweger[1]; *[1]Bruker Daltonics, Bremen, Germany*

WP 428 **Retention Time Prediction of Dansyl Labeled Tripeptides Using Machine Learning Methods for Dansylation LC-MS Metabolomics**; Hao Li[1]; Liang Li[2]; *[1]University of Alberta, Edmonton; [2]University of Alberta, Edmonton, AB*

WP 429 **Metabolite Classification into Major Chemical Classes using Supervised Machine Learning**; Elizabeth H Mahood; *Cornell University, Ithaca, NY*

WP 430 **A Scalable Approach to Curation of Public MS2 Spectra for Co-Analysis Using Untargeted Mass Spectrometry**; Alan K. Jarmusch[1,2]; Mingxun Wang[1,2]; Madeleine Ernst[1,2]; Ricardo R. da Silva[1,2]; Pieter C. Dorrestein[1,2]; *[1]Skaggs School of Pharmacy & Pharmaceutical Sciences, University of California – San Diego, La Jolla, CA; [2]Collaborative Mass Spectrometry Innovation Center, University of California – San Diego, La Jolla, CA*

WP 431 **MZmine 3 - a Comprehensive Mass Spectrometry Data Processing Framework for Metabolomics**; Tomáš Pluskal[1]; Robin Schmid[2]; Ansgar Korf[2]; Timothy R Fallon[1]; Aleksandr Smirnov[3]; Matej Orešič[1]; Xiuxia Du[3]; Jing-ke Weng[1]; *[1]Whitehead Institute for Biomedical Research, Cambridge, MA; [2]University of Muenster, Institute of Inorganic and Analytical Chemistry, Muenster, Germany; [3]The University of North Carolina at Charlotte, Charlotte, NC; [4]Örebro University, Örebro, Sweden*

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WP 432 **Improving Resolution of Frequency-Scanning ESI Ion Trap MS in Rough Vacuum using Periodic DC Focusing and Segment Quad Interface**; Jung-Lee Lin[1]; Hsi-Chang Shih[1]; Chung-Hsuan Chen[1]; *[1]The Genomics Research Center Academia Sinica, Taipei, Taiwan*

WP 433 **Software for Automated Laser Ablation and Capture from Tissue Sections**; Fabrizio Donnarumma[1]; Touradj Solouki[2]; Kermit K Murray[1]; *[1]Louisiana State University, Baton Rouge, LA; [2]Baylor University, Waco, TX*

WP 434 **Characterization of Quadrupol Mass Filters Regarding Elevated Entrance Ion Currents**; Markus Langner[1]; Marco Thinius[1]; Chris Heintz[1]; Yessica Brachthaeuser[2]; Hendrik Kersten[1]; Thorsten Benter[1]; *[1]Bergische Universität Wuppertal, Wuppertal, Germany; [2]Carl Zeiss SMT, Oberkochen, Germany*

WP 435 **Time-of-Flight Compensated Ion Transmission: Theory, Simulation, and Application in Fourier Transform Ion Cyclotron Resonance Mass Spectrometry**; Qinghao Wu[1]; Jared B. Shaw[2]; Ljiljana Pasa-Tolic[2]; *[1]IonX Tech, LLC, Richland, WA; [2]PNNL, Richland, WA*

WP 436 **Performance Evaluation of a Modified Quadropole Orbitrap Mass Spectrometer**; Tabiwang N. Arrey[1]; Rosa Jersie-Christensen Rakownikow[1]; Julia Kraegenbring[1]; Kerstin Strupat[1]; Markus Kellmann[1]; Catharina Crone[1]; Thomas Moehring[1]; Alexander Harder[1]; *[1]Thermo Fisher Scientific, Bremen, Germany*

WP 437 **Determining the Nature of MS Contamination with Various Sample Matrices**; Leigh Bedford[1]; Yang Kang[1]; Bradley B. Schneider[1]; Thomas R. Covey[1]; *[1]SCIEX, Concord, ON*

WP 438 **Reliable and Deep Proteome Coverage by Gas-Phase Fractionation of Peptides with a FAIMS Pro Interface on a Modified Quadrupole Orbitrap**; Julia Kraegenbring[1]; Tabiwang N. Arrey[2]; Michael W. Belford[3]; Satendra Prasad[3]; Kerstin Strupat[2]; Markus Kellmann[2]; Thomas Moehring[2]; Alexander Harder[2]; *[1]Thermo Fisher Scientific, Bremen, Germany; [2]Thermo Fisher Scientific, Bremen, Germany; [3]ThermoFisher, San Jose, CA*

WP 439 **Development of Vacuum Measurement and Control System for Quadrupole Mass Spectrometer**; Li Kai[1]; li ming[1]; *[1]NCS Testing technology Co.,Ltd, Beijing, China*

WP 440 **Development of Universal and High Sensitivity Ion Mobility Spectrometer with APCI Ion Source for HPLC (LC-APCI-IMS)**; Yoshinori Arita[1]; Akiko Imazu[1]; Motohide Yasuno[1]; Hiroshi Tanaka[1]; Toshiya Habu[1]; Yoshihito Yuasa[1]; Kiyoshi Ogawa[1]; *[1]Shimadzu Corporation, Kyoto, Japan*

WP 441 **DRy Ion Localization and Locomotion (DRILL) MS Interface for Sensitivity Enhancement via Droplet Size Based Inertial Separation**; Jung Lee[1]; Peter Kottke[1]; Crystal L Pace[2]; David C Muddiman[2]; Alex Jonke[3]; Matthew P. Torres[3]; Andrei Fedorov[1]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]North Carolina State University, Raleigh, NC; [3]School of Biological Sciences, Georgia Institute of Technology, Atlanta, GA*

WP 442 **Ion Manipulation Using Stacked PCB-Based Electrode Device (SPED)**; Yi-teng Hsiao[1]; Szu-Wei Chou[1]; Yi-Kun Lee[1]; Pin-Duo Lee[1]; Shih-Chieh Yang[1]; Yao-Hsin Tseng[1]; Chun-Yen Cheng[1]; *[1]AcroMass Technologies, Inc., Hsinchu, Taiwan*

WP 443 **Comparison of UPLC and RapidFire MS/MS Methods for Content Uniformity Analysis in Tablet-Splitting for a Narrow Therapeutic Index Drug Warfarin**; Jiang Wang[1]; Haiou Qu[2]; Robert L Hunt[2]; Leanna Hengst[2]; Patrick J. Faustino[2]; Jinhui Zhang[2]; *[1]Food and Drug Administration - Center for Drug Evaluation and Research, Silver Spring, Md; [2]FDA, Silver Spring, MD*

WP 444 **Impact of Dwell Time and Ion Flux on Multiple Reaction Ion Monitoring (MRM) Measurement Precision**; Behrooz Zekavat[1]; Charles Nichols[1]; Anabel Fandino[1]; *[1]Agilent Technologies, Santa Clara, CA*

WP 445 **Resolution Improvement through Modulation of Collective Ion Motion and Ejection in Quadrupole Ion Trap Mass Spectrometry for Intact Protein**; Yi-teng Hsiao[1]; Szu-Wei Chou[1]; Shih-Chieh Yang[1]; Pin-Duo Lee[1]; Yi-Kun Lee[1]; Yao-Hsin Tseng[1]; Chun-Yen Cheng[1]; *[1]AcroMass Technologies, Inc., Hsinchu, Taiwan*

WP 446 **A Novel Mass Spectrometry-Based Analytical System for Single-Cell Proteomics and Metabolomics in Mammalian Cells**; Yoshihiro Izumi[1]; Kousuke Hata[1]; Kohta Nakatani[1]; Takeshi Hara[1]; Shohei Yamamura[2]; Masaki Matsumoto[1]; Takeshi Bamba[1]; *[1]Medical Institute of Bioregulation, Kyushu University, Fukuoka, Japan; [2]Health Research Institute, National Institute of Advanced Industrial Science and Technology, Kagawa, Japan*

WP 447 **Transfer of Plasma-Generated Ions into a Fourier Transform Quadrupole Ion Trap (FT-QIT) with Running RF Trapping Field**; Yessica Brachthäuser[1]; Chris Heintz[2]; Alexander Laue[1]; Michel Aliman[1]; Hin Yiu Chung[1]; Thorsten Benter[2]; *[1]Zeiss SMT GmbH, Oberkochen, Germany; [2]University of Wuppertal, Wuppertal, Germany*

WP 448 **Automated Tuning of an Electromagnetostatic Cell for Electron Capture Dissociation with Q-ToF Mass Spectrometers**; Blake A. Hakkila[1]; Joseph C. Meeuwsen[1,2]; Yury V. Vasil'ev[1,2]; Joseph S. Beckman[1,2]; Valery G. Voinov[1,2]; *[1]e-MSion, Inc., Corvallis, OR; [2]Oregon State University, Corvallis, OR*

WP 449 **Rectilinear Quadrupole Ion Guides: Transmission as a Function of Mass, RF Amplitude and RF Frequency**; Kevin Kuchta[1]; Luke J. Metzler[2]; Michael J. Van Stipdonk[2]; Randall E Pedder[1]; *[1]Ardara Technologies, Ardara, PA; [2]Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA*

WP 450 **Developing a Multi-Pass Overtone Mobility Spectrometry "Ping Pong" Insert to Improve the Drift Resolution of the Waters HDMS (G1)**; Kyle Buckley[1]; Marc Legris[1]; Arthur Laganowsky[2]; David H. Russell[2]; David E. Clemmer[1]; *[1]Indiana University, Bloomington, IN; [2]Texas A&M University, College Station, TX*

WP 451 **Characterization of Ion Funnels: Transmission Characteristics as a Function of Mass, RF Voltage and RF Frequency**; Luke J. Metzler[1]; Kevin Kuchta[2]; Michael J. Van Stipdonk[1]; Randall E Pedder[2]; *[1]Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA; [2]Ardara Technologies L.P., Ardara, PA*

WP 452 **Modifying the Ion Optics and Scan Sequences on a Tribrid MS to Improve Sensitivity, Duty Cycle, and Overall Instrument Ease-of-Use**; Graeme McAlister[1]; Michael Goodwin[1]; Lee Earley[1]; Raman Mathur[1]; Oliver Lange[2]; Romain Huguet[1]; Vlad Zabrouskov[1]; Mike Senko[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Bremen, Germany*

INSTRUMENTATION: NEW CONCEPTS
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WP 453 **A Microchannel Thermalization Inlet Design to Eliminate Impact-Induced Molecular Fragmentation in Closed-Source Mass Spectrometers**; Brandon Turner[1]; Anupriya Anupriya[1]; Sandra Osburn-Staker[1]; Abraham De la Cruz[1]; Eric T. Sevy[1]; Daniel E. Austin[1]; *[1]Brigham Young University, Provo, UT*

WP 454 **Concurrent Dual Polarity Ion Mobility (IM) Separations using Traveling Wave-based Structures for Lossless Ion Manipulations (SLIM)**; Isaac Kwame Attah[1]; Yehia M. Ibrahim[1]; Sandilya V.B. Garimella[1]; Gabe Nagy[1]; Randolph V. Norheim[1]; Colby E. Schimelfenig[1]; Richard D. Smith[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

WP 455 **Ion Mobility Measurement using a Miniature Dual-Trap Mass Spectrometer**; Jingjin Fan[1]; Xinwei Liu[1]; Xiaoyu Zhou[1]; Zheng Ouyang[1]; *[1]Tsinghua University, Beijing, China*

WP 456 **Combining DIUTHAME and Stigmatic-Type Mass Microscope toward Cellular Scale Imaging Mass Spectrometry**; Tsuyoshi Hirao[1,2]; Yasuhide Naito[1]; *[1]GPI, Hamamatsu, Japan; [2]Hamamatsu Photonics K.K., Hamamatsu, Japan*

WP 457 **High Sensitivity and Resolution IMS Separations at 100% Ion Utilization Efficiency**; Sandilya Garimella[1]; Gabe Nagy[1]; Yehia M Ibrahim[1]; Isaac K. Attah[1]; Aneesh Prabhakaran[1]; Richard D. Smith[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

WP 458 **Bridging the Gap Between Gas- and Condensed-Phase Using Dual-Polarity Ion Soft Landing**; Pei Su[1]; Hang Hu[1]; Jonas Warneke[1]; Mikhail Belov[2]; Gordon Anderson[3]; Julia Laskin[1]; *[1]Purdue University, West Lafayette, IN; [2]Spectroglyph, LLC, Kennewick, WA; [3]GAA Custom Engineering, LLC, Benton City, WA*

WP 459 **Determination of Drugs of Abuse in Human Hair by On-Line Supercritical Fluid Extraction – Supercritical Fluid Chromatography - Mass Spectrometry**; Alison P Wicker[1]; Blair K Berger[1]; Tairo Ogura[2]; Kenichiro Tanaka[2]; Masayuki Nishimura[3]; Vivian chen[3]; William Hedgepeth[3]; Kevin A. Schug[1]; *[1]University of Texas at Arlington, Arlington, TX; [2]Shimadzu Corporation, Nakagyo-ku, Japan; [3]Shimadzu Scientific Instruments, Inc, Innovation Center, Columbia, MD*

WP 460 **Implementation of an Ambient-Fourier Transform-Drift Tube on an Ultra High Mass Range Orbitrap™ Mass Spectrometer for Analysis of Protein Complexes**; Sarah Sipe[1]; James Sanders[1]; Tobias Reinecke[2]; Brian H. Clowers[2]; Jennifer S Brodbelt[1]; *[1]Department of Chemistry, University of Texas at Austin, Austin, TX; [2]Department of Chemistry, Washington State University, Pullman, WA*



WP 461 **Evaluation of a Novel PTR-TOFMS Setup Capable of Extremely Rapid Reagent Ion Switching**; Alfons Jordan[1]; Christian Lindinger[1]; Stefan Feil[1]; Gernot Hanel[1]; Lukas Märk[1]; Philipp Sulzer[1]; *[1]IONICON Analytik GmbH., Innsbruck, Austria*

WP 462 **Experimental Design of a Rotor-Induced Collision Cell (RICC) to Study Molecular Fragmentation During Hypervelocity Impacts Prior to Mass Analysis**; Abraham L De la Cruz Hernandez[1]; Friso Van Amerom[2]; Anupriya Anupriya[3]; Sandra Osburn-Staker[4]; Brandon Turner[1]; Eric T. Sevy[1]; Daniel E. Austin[1]; *[1]Brigham Young University, Provo, UT; [2]Mini Mass Consulting, St. Petersberg, Florida; [3]Intel, Portland, Oregon; [4]University of Utah, Salt Lake City, UT*

WP 463 **Pulse Width Modulation Control of Electron Beam Intensity in Electron Capture Dissociation using Precursor Charge State Information**; Anjali Chelur[1]; Suya Liu[1]; Calin Bradau[1]; Pavel Ryumin[1]; Thomas J Binko[1]; Nick Albeanu[1]; Takashi Baba[1]; *[1]SCIEX, Concord, ON*

WP 464 **High Resolution Acceptance Phase Plane Analysis of the Rectangular and Sinusoidally Driven Linear RF Quadrupole**; Adam P. Huntley[1]; Gregory F. Brabeck[2]; Peter T. A. Reilly[1]; *[1]Washington State University, Pullman, WA; [2]Excellims Corporation, Acton, Massachusetts*

WP 465 **SLIMion: An Automated Framework for Performing Multi-Dimensional Parameter Optimizations of Structures for Lossless Ion Manipulations (SLIM) Using SIMION**; Ron Danehy[1]; Ahmed M Hamid[1]; Liulin Deng[1]; John Daniel Debord[1]; *[1]MOBILion Systems Inc., Exton, PA*

WP 466 **A Novel Instrument Platform for the Investigation of Particle Formation from the Gas Phase**; Tina Kasper[1]; Martin Hoener[1]; Dimitris Papanastasiou[2]; Alexander Lekkas[2]; Diamantis Kounadis[2]; John Orfanopoulos[2]; *[1]University of Duisburg, Duisburg, Germany; [2]Fasmatech, Athens, Greece*

WP 467 **Covalent Modification via Ion/Ion Reactions with Ion Mobility/Mass Spectrometry Structural Analyses**; Veronica V Carvalho[1]; Ian K. Webb[1]; *[1]IUPUI Department of Chemistry & Chemical Biology, Indianapolis, IN*

WP 468 **Development of Colinear Resonance Ionisation Spectroscopy (CRIS) for Sub-ppt quasi-IRMS Based Assays Including Carbon Dating**; Giles Edwards[1,2]; Ben Cooper[1]; Sultan Alsufyani[1]; Christopher Ricketts[1]; Holly Perrett[1]; Cory Binnersley[1]; Kieran Flanagan[1,2]; *[1]The University of Manchester, School of Physics and Astronomy, Manchester, United Kingdom; [2]The Photon Science Institute, The University of Manchester, Manchester, United Kingdom*

WP 469 **Extended Path Length Ion Mobility with Structures for Lossless Ion Manipulations (SLIM) as an Ultra-Sensitive Pressure Gauge**; Gregory Webster[1]; Ahmed Mohamed Hamid[1]; Daniel DeBord[1]; Liulin Deng[1]; Kelly Wormwood[1]; Anisha Yadav[1]; Gordon Anderson[2]; *[1]MOBILion Systems Inc., Exton, PA; [2]GAA Custom Engineering, LLC, Benton City, WA*

WP 470 **Development of a [CID-TIMS]x[CID-TIMS]-q-CID-TOF HRMS platform for Discovery and Targeted o-mics Studies**; Mark E. Ridgeway[1]; Melvin A. Park[2]; Francisco Fernandez Lima[3]; *[1]Bruker Daltonics Inc., Billerica, MA; [2]Bruker Daltonics Inc., Billerica, MA 01821; [3]Florida International University, Miami, FL*

WP 471 **Phasing two-dimensional (2D) Fourier transform ion cyclotron resonance mass spectrometry (FT-ICR MS) in both dimensions**; Ulviya Abdulkarimova[1]; Marc Haegelin[2]; Fabrice Bray[2]; Anne Jeannin-Girardon[1]; Pierre Collet[1]; Christian Rolando[2]; *[1]Université de Strasbourg, Strasbourg, France; [2]Université de Lille, Villeneuve d'Ascq, France*

WP 472 **Neoteric Approaches to MS Instrumentation Facilitated by Simulation**; Jerome Moore; *Robot Nose Corporation, Lemont, IL*

WP 473 **Ruthenium Catalyzed 2e-/2H+ PCET - Characterizing the Catalyst-Substrate Interaction with High-Resolution Mass Spectrometry and Gas-Phase Vibrational Spectroscopy**; Fabian S Menges[1]; Evan H Perez[1]; Mauricio Cattaneo[2]; James Mayer[1]; Mark Johnson[1]; *[1]Yale University, New Haven, CT; [2]Universidad Nacional de Tucumán, Tucumán, Argentina*

WP 474 **Improved Integration of a Separation Column to an Ion Source for Liquid Chromatography Mass Spectrometry**; Michael Fogwill[1]; Angela Doneanu[1]; Stephen Hattan[1]; Jason Hill[1]; Wade P Leveille[1]; Thomas McDonald[1]; Joseph Michienzi[1]; *[1]Waters Corporation, Milford, MA*

WP 475 **Nano-Scale HPLC System for Isocratic and Gradient Ultra-Nano HPLC Separations**; Stan Stearns[1]; Jennifer Copeland[1]; Huamin Cai[1]; Martin Brisbin[1]; Alex Plistil[1]; Hal Barnett[1]; *[1]VICI Valco Instrument, Houston, TX*

WP 476 **Advanced analytics for regulatory science: Application of an innovative robotic sample separation system coupled with tandem mass spectrometry**; Jinhui Zhang[1]; Patrick J. Faustino[1]; *[1]FDA, Silver Spring, MD*

WP 477 **Growing MS adoption: A "Self-Driving" Mass Spectrometer Designed for Non-MS Experts**; Maggie A. Ostrowski[1]; F. Robert Ley[1]; Kyle Covert[1]; Kai Zhang[1]; Susan Shen[1]; Shane E. Tichy[1]; *[1]Agilent Technologies, Inc., Santa Clara, CA*

WP 478 **Automated and Simultaneous Identification and Quantification in Extractables and Leachables Analysis**; Andrew Jones[1]; Tommy Saunders[1]; Ashley Baeten[2]; Yongdong Wang[3]; *[1]Activated Research Company, Eden Prairie, MN; [2]Abbott, St. Paul, Minnesota; [3]Cerno Bioscience, Norwalk, CT*

ION MOBILITY: APPLICATIONS II
479-500

WP 479 **Computational Chemistry and Ion Mobility – Mass Spectrometry at High Resolving Power Suggest Prototropism of Cyclic Lipopeptides**; Andréa Mccann[1]; Christopher Kune[1]; Johann Far[1]; Philippe Massonnet[1,2]; Philippe Jacques[3]; Marc Ongena[3]; Loïc Quinton[1]; Edwin De Pauw[1]; *[1]University of Liege, MS Lab - GIGA, MolSys Research Unit, Liege, Belgium; [2]Maastricht Multimodal Molecular Imaging (M4I) Institute, Division of Imaging Mass Spectrometry, Maastricht, Netherlands; [3]Terra teaching and research center, Gembloux Agro-Bio Tech, University of Liege, Gembloux, Belgium*

WP 480 **Use of DESI with IMS Enhancement in Study of Transferred Material on Paper**; Liepin Huang[1]; Carrie L Hogue[2]; Gilbert Castillo[2]; *[1]Corning Inc.,, Horseheads, NY; [2]Corning Inc., Painted Post, 14870*

WP 481 **Collision Induced Unfolding Experiments to Decipher the Structural Regions of a Hybrid Monoclonal Antibody.**; Thomas Botzanowski[1]; Oscar Hernandez-Alba[1]; Olivier Colas[2]; Elsa Wagner-Rousset[2]; Alain Beck[2]; Sarah Cianferani[1]; *[1]Laboratoire de Spectrométrie de Masse BioOrganique, Université de Strasbourg, CNRS, IPHC UMR 7178, Strasbourg, France; [2]IRPF, Centre d'Immunologie Pierre-Fabre (CIPF), Saint-Julien-en-Genevois, France*

WP 482 **New High Resolution Mass Spectrometry Ion Mobility Applications in the Identification of Challenging Environmental Metabolites**; Yelena A. Adelfinskaya[1]; David G McCaskill[1]; Jesse L Balcer[1]; Nick N Wang[1]; Jeffery Gilbert[1]; Michael W. Madary[1]; Pete L. Johnson[1]; Suresh Annangudi Palani[1]; Scott A. Greenwalt[1]; *[1]Corteva Agriscience, Indianapolis, IN*

WP 483 **Characterisation of Intact Hemoglobin Variants Utilising a Cyclic Ion Mobility-Enabled Quadrupole Time-of-Flight (Q-cIM-oaToF) Mass Spectrometer**; Ahmad Alkawi[1]; James Scrivens[1]; Gillian Taylor[1]; Safwan Akram[1]; Martin Palmer[2]; Jakub Ujma[2]; Kevin Giles[2]; Jonathan P Williams[2]; Matthew Edgeworth[3]; *[1]Teesside University, Middlesbrough,*

United Kingdom; [2]Waters Corportaion, Cheshire, United Kingdom; [3]MedImmune, Granta Park, United Kingdom

WP 484 **Copper Complexation Strategies for Differentiating Amino Acid Enantiomers by Ion Mobility**; Emanuel Zlibut[1]; Jody C. May[1]; John A. McLean[1]; *[1]Vanderbilt University, Nashville, TN*

WP 485 **Chirality-Regulated Human Serum Albumin-Neuropeptide Interactions Revealed by Ion Mobility-Mass Spectrometry**; Jiabao Guo[1]; Gongyu Li[2]; Lingjun Li[1,2]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]School of Pharmacy, University of Wisconsin-Madison, Madison, WI*

WP 486 **Structural Analysis of Phosphopeptide Conformers using ECD, TWIMS and Molecular Modelling**; Anna L. Simmonds[1]; Andrea F Lopez-Clavijo[2]; Peter J Winn[1]; John K Heath[1]; David H. Russell[3]; Iain B. Styles[1]; Helen J Cooper[1]; *[1]University of Birmingham, Birmingham, United Kingdom; [2]Babraham Institute, Cambridge, United Kingdom; [3]Texas A&M University, College Station, TX*

WP 487 **Analysis of Heteroatomic Species in Weathered Crude Oil using Ion Mobility Time-of-Flight ESI-MS**; Nolan Snyder[1]; Feiyue Wang[1]; Jake Ritchie[1]; Diana Saltymakova[1]; Katarzyna Polcwiartek[1]; Durell S. Desmond[1]; Casey Hubert[2]; Gary A. Stern[1]; Alastair F. Smith[2]; *[1]University of Manitoba, Winnipeg, MB; [2]University of Calgary, Calgary, AB*

WP 488 **Analysis of Gold-Molybdenum Complexes by Nano-Electrospray Ionization-Ion Mobility-Mass spectrometry**; Hannah J Harbin[1]; Kyle L Wilhelm[1]; Dhirgam Humaidy[2]; Raul Villacob[1]; Alice E Bruce[2]; Mitchell R. M. Bruce[2]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX; [2]The University of Maine, Orono, ME*

WP 489 **Improvement in Quantitative Analysis of Vitamin D Metabolites in Blood using Click Derivatization Reagents Combined with LC-TimsTOF**; Debin Wan[1]; Xuejun Peng[2]; Jun yang[1]; Bogdan Barnych[1]; Nalin Singh[1]; Bruce D Hammock[1]; *[1]UC Davis, Davis, CA; [2]Bruker Daltonics Inc., San Jose, CA*

WP 490 **Azobenzene Photoswitches: Observing Molecules Switching Using Ion Mobility Mass Spectrometry**; Julien De Winter[1]; Agostino Galanti[2]; Quentin Duez[1]; Jérôme Cornil[1]; Paolo Samori[2]; Pascal Gerbaux[1]; *[1]University of Mons, Mons, Belgium; [2]University of Strasbourg, Strasbourg, France*

WP 491 **Enhanced Software for the Classification of Charge Multiplexed Collision Induced Unfolding Data**; Daniel A. Polasky[1]; Sugyan M. Dixit[1]; Kathryn D. Kulju[1]; Daniel D. Vallejo[1]; Ruwan T. Kurulugama[2]; John C. Fjeldsted[2]; Brandon T. Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI; [2]Agilent Technologies, Santa Clara, CA*

WP 492 **The Benefit of Peptide CCS Value Prediction and Experimental Determination**; Sebastian Wehner[1]; Favio Salinas[2]; Stuart Pengelley[1]; Heiko Neuweger[1]; Heiner Koch[1]; Anjali Alving[3]; Na Parra[3]; Greig Michael[3]; Juergen Cox[2]; Detlev Suckau[1]; *[1]Bruker Daltonics, Bremen, Germany; [2]Max Planck Institute of Biochemistry, Martinsried, Germany; [3]Bruker Daltonics Inc., Billerica, MA*

WP 493 **Characterization of Derivatized Carbohydrates Using High Resolution Cyclic IMS and Tandem-IMS Techniques**; Kristin McKenna[1]; Andrew Baker[2]; Martin Palmer[3]; Dale Cooper-Shepherd[3]; Facundo M. Fernandez[1]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]Waters Corporation, Pleasanton, CA; [3]Waters Corporation, Wilmslow, United Kingdom*

WP 494 **Differentiating Commercial Lubricant Oils using Ion-Mobility Enabled Mass Spectrometry**; Jeff Goshawk[1]; Eleanor Riches[1]; Caitlyn Da Costa[1]; Gordon Jones[1]; *[1]Waters Corporation, Wilmslow, United Kingdom*

WP 495 **Development of a Collisional Cross Section Library using Trapped Ion Mobility Spectrometry (TIMS) and Its Use in Plant Metabolomics**; Mark J Schroeder[1,2,3]; Sven W. Meyer[4]; Aiko Barsch[4]; Lloyd W. Sumner[1,2,3]; *[1]Department of Biochemistry, University of Missouri, Columbia, MO; [2]Bond Life Sciences Center, University of Missouri, Columbia, MO; [3]Interdisciplinary Plant Group, University of Missouri, Columbia, MO; [4]Bruker Daltonik GmbH, Bremen, Germany*

WP 496 ***De Novo* Peptide Sequencing Using TIMS- MS/MS for Amphibian Skin Peptides**; Benjamin Bokor[1]; Jacob Porter[1]; Mario E. Gomez Hernandez[1]; Alessandro Catenazzi[1]; Francisco A. Fernandez-Lima[1]; *[1]Florida International University, Miami, FL*

WP 497 **Post-ionization separation of isomeric cannabinoids by means of Trapped Ion Mobility-Mass Spectrometry**; Arne Behrens[1]; Sabrina Kröger[1]; Uwe Karst[1]; *[1]University of Muenster, Institute of Inorganic and Analytical Chemistry, Muenster, Germany*

WP 498 **Atmospheric Pressure Ion-Mobility MS with a Low Entrance Potential**; William P. McMahon[1]; Joseph E. Lesniewski[1]; Kaveh Jorabchi[1]; *[1]Georgetown University, Washington, DC*

WP 499 **Trapped Ion Mobility Spectrometry and Surface-Induced Dissociation (TIMS-SID) on a 15 T FT-ICR for Structural Characterization of Native Protein Complexes**; Erin Panczyk[1,2]; Arpad Somogyi[2,3]; Mark E. Ridgeway[4]; Melvin A. Park[4]; Vicki H. Wysocki[1,2,3]; *[1]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; [2]Resource for Native MS Guided Structural Biology, The Ohio State University, Columbus, OH; [3]Campus Chemical Instrument Center, Mass Spectrometry and Proteomics Facility, The Ohio State University, Columbus, OH; [4]Bruker Daltonics Inc., Billerica, MA*

WP 500 **Exploring the Conformational Space of Growth Hormone-Releasing Hormone Analogs using Dopant Assisted Trapped Ion Mobility Spectrometry**; Javier Moreno[1]; Kevin Jeanne Dit Fouque[1]; Francisco Fernandez-Lima[1]; *[1]Florida International University, Miami, FL*

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501-517

WP 501 **Direct LC/MS Analysis Method of Surfactants Contained in Antibody Drugs Using a Polymer-Based Reversed Phase Column**; Leah Sullivan[1]; Junji Sasuga[1]; Hiroki Takenaka[1]; Eiji Kagawa[1]; Ron Benson[1]; *[1]Shodex, Showa Denko America, Inc., New York, NY*

WP 502 **Mutant KRas Protein and Tryptic Peptides Separation and Characterization Using Enhanced Fluidity Liquid Chromatography Coupled with Tandem Mass Spectrometry**; Juan Bian; *The Ohio State University, Columbus, OH*

WP 503 **Ultra-fast Capillary-Flow LC-MS Profiling of Complex Biological Matrices: Applicable to Large Sample Cohorts**; Oleksandr Boychenko[1]; Jenny Ho[2]; Christopher Pynn[1]; *[1]Thermo Fisher Scientific, Germering, Germany; [2]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom*

WP 504 **The Characterization of Column Heating Effect in Nano-Flow Liquid Chromatography Mass Spectrometry (nanoLC-MS)-Based Proteomics**; Linhui Zhai[1]; Bolin Li[1]; Hao Hu[1]; Fang Guo[2]; Ping Liu[1]; Minjia Tan[1]; *[1]Shanghai Institute of Materia Medica, Chinese Academy of Sciences, Shanghai, China; [2]Shanghai Easymass Co., Ltd., Shanghai, China*

WP 505 **Characterization of the Merck Sample Collection by UPLC-MS And Evaluation of the Data Using Virscidian**; Wilfredo Pinto; *Merck, Rahway, NJ*

WP 506 **An Updated Perspective on Deconvoluting Chimeric MS/MS Spectra by LC and Precursor Isolation and Their Subsequent Assignment by CharmeRT**; Manuel I. Villalobos Solis[1,2]; Richard J. Giannone[1]; Robert L. Hettich[1]; Paul E. Abraham[1]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN; [2]University of Tennessee, Knoxville, TN*

WP 507 **Rapid Separation of Reduced Antibody Chains by Size Exclusion Chromatography Coupled to Electrospray Mass Spectrometry**; John H. Robinson[1]; John O. Hui[1]; Iain D. G. Campuzano[1]; *[1]Amgen Inc., Thousand Oaks, CA*

WP 508 **Instrument Performance Evaluation and Tracking Using a Quality Control Standard for Proteomics Laboratory**; Shenheng Guan[1, 2]; Jonathan Krieger[2]; Leanne Wybenga-Groot[2]; Bin Ma[3]; Michael F. Moran[2, 4]; *[1]University of Waterloo, Waterloo; [2]SPARC BioCentre, Hospital for Sick Children, Toronto, Ontario; [3]University of Waterloo, Waterloo, ON; [4]University of Toronto, Toronto, ON*

WP 509 **Characterization of the Activity and Kinetics of Guanine Deaminase**; Justin Godinho[1]; Ben Libert[1]; Barry Boyes[1]; *[1]Advanced Materials Technology, Wilmington, DE*

WP 510 **A new LC-MS Approach for Synthetic Peptide Characterization and Impurity Profiling**; Asish Chakraborty[1]; Nilini Nilini Ranbaduge[1]; Ying Qing Yu[1]; *[1]Waters Corporation, Milford, MA*

WP 511 **Becoming Street-Smart in the CDMO Space: Utilization of Multiple Technologies to Harmonize Release and Characterization Assays for non-mAb Proteins**; Irina Perdivara[1]; Margo Wilson[1]; Clara Smith[1]; *[1]Fujifilm Diosynth Biotechnologies, Morrisville, NC*

WP 512 **Intact Analysis of Biopharmaceuticals by Hydrophobic Interaction/Reversed Phase 2D-LC/MS System**; sandeep kondaveeti[1]; Dat Phan[1]; Bob Giuffre[1]; Gregory Staples[2]; Andrew Coffey[3]; Suma Ramagiri[1]; Priya Jayaraman[1]; Jin Zhang[1]; *[1]Agilent Technologies, Inc., Wilmington, DE; [2]Agilent Technologies, Inc., Santa Clara, CA; [3]Agilent Technologies, Chruch Stretton, United Kingdom*

WP 513 **A Quantitative Compliant Multi Attribute Methodology (MAM) LC/MS workflow**; Zoe Zhang[1]; Sean McCarthy[2]; Elliott Jones[1]; Todd Stawicki[2]; *[1]Sciex, Redwood City, CA; [2]Sciex, Framingham, MA*

WP 514 **A Sensitive Microflow LC/MS/MS Method for the Analysis of Corticosteroids in Human Plasma**; Ting Liu[1]; Wenhai Jin[1]; Daniel K Blake[2]; *[1]Sciex, Shanghai, China; [2]SCIEX, Warrington, United Kingdom*

WP 515 **Homology-Based Peptide Retention Time Prediction for Proteomic RP HPLC-MS Applications**; Oleg V. Krokhin[1]; Vic Spicer[1]; *[1]University of Manitoba, Winnipeg, MB*

WP 516 **Temperature-Specific Peptide Retention Time Prediction for nano-RP-HPLC in Proteomic Applications**; Carina Villacres[1]; Benilde Mizero[2]; Vic Spicer[3]; Rosa Viner[4]; Julian Saba[5]; Bhavin Patel[6]; Sergei Snovida[6]; Penny Jensen[6]; Andreas Huhmer[4]; Oleg V. Krokhin[2, 3, 7]; *[1]Manitoba Centre for Proteomics and Systems Biology, University of Manitoba, Winnipeg, Manitoba; [2]Department of Chemistry, University of Manitoba, Winnipeg, MB; [3]Manitoba Centre for Proteomics and Systems Biology, University of Manitoba, Winnipeg, MB; [4]Thermo Fisher Scientific, San Jose, CA; [5]Thermo Fisher Scientific, Mississauga, ON; [6]Thermo Fisher Scientific, Rockford, IL; [7]Department of Internal Medicine, Winnipeg, MB*

WP 517 **Peptide Retention Time Prediction for TMT-Labeled Peptides in RP-HPLC for Proteomic Applications**; Benilde Mizero[1]; Carina Villacres[2]; Vic Spicer[2]; Rosa Viner[3]; Julian Saba; Bhavin Patel[4]; Sergei Snovida[4]; Penny Jensen[4]; Andreas Huhmer[3]; Oleg V. Krokhin[2]; *[1]Department of Chemistry, University of Manitoba, Winnipeg, MB; [2]Manitoba Centre for Proteomics and Systems Biology, University of Manitoba, Winnipeg, Manitoba; [3]ThermoFisher, San Jose, CA; [4]Thermo Fisher Scientific, Rockford, IL*

LC/MS: SAMPLE PREPARATION I
518-542

WP 518 **Simultaneous Extraction of Proteins, Lipids, and Metabolites for Integrated-omics Approaches for Low Tissue Sampling Volumes**; Luke T. Richardson[1]; Amy N. W. Schnelle[1]; Fabrizio Donnaruma[2]; Michael E. Pettit[1]; Shubhneet Warar[1]; Nicholas M. von Waaden[1]; Kermit K. Murray[2]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX; [2]Louisiana State University, Baton Rouge, LA*

WP 519 **A Comparative Analysis of Two Sample Preparation Methods for the Multi-Omic Analysis of Proteins, Lipids, and Metabolites**; Melissa R Pergande[1, 2]; Sheher Banu Mohsin[2]; Limian Zhao[3]; Stephanie M Cologna[1]; *[1]University of Illinois at Chicago, Chicago, IL; [2]Agilent Technologies, Wood Dale, IL; [3]Agilent Technologies, Inc., Wilmington, DE*

WP 520 **A Robotic System for High Throughput Isolation of Phospholipids from Non-Polar Lipids**; Hui Gyu Park[1]; Jeffery G. McDonald[2]; Bonnie M. Thompson[2]; Gonçalo Vale[2]; Tom Brenna[1]; *[1]University of Texas at Austin, Austin, TX; [2]University of Texas Southwestern Medical School, Dallas, Texas*

WP 521 **Phospholipid Removal from Protein Precipitated Plasma Using In-Line Sample Preparation (ILSP)**; Sharon Lupo[1]; Randy Romesberg[1]; Xiaoning Lu[1]; *[1]Restek, Bellefonte, PA*

WP 522 **Study of Co-Extracted Matrix Impurities on Coated Solid Phase Microextraction Devices During Short Extractions Out of Plasma**; Olga I. Shimelis[1]; Katherine K. Stenerson[1]; Teresa Marsala[1]; Emily R. Barrey[1]; Hugh Cramer[1]; Cory Muraco[1]; *[1]MilliporeSigma, Bellefonte, PA*

WP 523 **A Sensitive LC-MS/MSMethod for Quantitation of Free and Liposomal Doxorubicin in Dog Plasma**; Sheng Wang[1]; Jing Huang[1]; Yifan Wang[1]; Lele Yu[1]; Xiaoying Jin[1]; Dawei Zhou[2]; *[1]Lab Testing Division of WuXi AppTec, Inc., Suzhou Site, Suzhou, China; [2]WuXi AppTec, Cranbury, NJ*

WP 524 **LC-MS/MS Method for Determining Cannabidiol in Complex Matrices with a Dual Column-Switching Strategy**; Ze Li[1]; Peng Wang[1]; *[1]WuXi AppTec, Plainsboro, NJ*

WP 525 **Determination of Tetramethylammonium Hydroxide in Serum by micro Solid Phase Extraction Coupled to Liquid Chromatography-Tandem Mass Spectrometry**; Chung-Yu Chen[1]; Chia-Ying Lin[1]; Cheng-Chieh Yen[2]; Maw-Rong Lee[1]; *[1]National Chung-Hsing University, Taichung, Taiwan; [2]Chung Shan Medical University, Taichung, Taiwan*

WP 526 **Development and Implementation of Ultra-Trace Level Detection by LC/MS/MS for Quantitation of Thyroxine Isomers and Metabolites for *in-vitro* Toxicology Screening**; Jeremy McFadden[1]; Mercedes Biven[1]; David Robbins[2]; Jessica LaRocca[1]; Audrey Lehman[1]; Bethany Hannas[1]; David Hills[2]; *[1]Corteva Agriscience, Indianapolis, IN; [2]Eurofins Lancaster Laboratories Professional Scientific Services, Lancaster, PA*

WP 527 **Automating the Analysis of Estrogens in Plasma using a Multi-Purpose Auto-Sampler Coupled to Liquid Chromatography Triple Quadrupole Mass Spectrometry**; Mary Blackburn; *Thermo Fisher Scientific, San Jose, CA*

WP 528 **Evolution of Sample Preparation: Workflow Simplification Utilizing Sample Hold-Up Technology in Forensic and Clinical Analyses**; Rhys Jones[1]; Adam Senior[1]; Helen Lodder[1]; Lee Williams[1]; Geoff Davies[1]; Katie-Jo Teehan[1]; Alan Edgington[1]; Steve Jordan[1]; Claire Desbrow[1]; Paul Roberts[1]; *[1]Biotage GB Limited, Cardiff, United Kingdom*

WP 529 **Determination of Optimal Sample Size with Microelution without Dry Down Using Solid Phase Extraction for a Drugs of Abuse Panel**; Jillian Neifeld[1]; Jeremy Smith[1]; Stephanie Marin[1]; Mohamed Youssef[1]; Elena Gairloch[1]; *[1]Biotage, Charlotte, NC*

WP 530 **A new device for direct QuEChERS salts extraction: Application to Drugs of Abuse in Blood, Urine and Oral Fluid**; Tiphaine Robin[1]; Stephane Moreau[2]; Franck Saint-Marcoux[1]; Etienne Maout[3, 3]; *[1]CBRS, Limoges, France; [2]Shimadzu Europa GmbH, Duisburg, Germany; [3]shimadzu france, Paris, France*

WP 531 **UHPLC-MS/MS Analysis of Neonicotinoids and their Metabolites in Plant Tissues and Pollen by Modified QuEChERS**; Viet D Dang[1]; Maura J Hall[1]; Ed George[2]; David J. Borts[1]; *[1]Iowa State University, Ames, IA; [2]ThermoFisher Scientific, San Jose, CA*

WP 532 **Determination of Pesticides in Edible Oils by GC-MS/MS**; Euan Ross[1]; Jd De-Alwis[1]; Simon Hird[1]; Kenneth Rosnack[2]; *[1]Waters, Wilmslow, United Kingdom; [2]Waters Corporation, Milford, MA*

WP 533 **Determination of Pesticides in Dog Collars by On-line Supercritical Fluid Extraction – Supercritical Fluid Chromatography - Mass Spectrometry**; William Hedgepeth[1]; Yuka Fujita[2]; *[1]Shimadzu Scientific Instruments, Inc, Columbia, MD; [2]Shimadzu Scientific Instruments, Inc., Columbia, Maryland*

WP 534 **Future Directions of Extractable and Leachable (E/L) Analysis from Automated Sample Preparation using online SPE and Online Solvent Mixing**; David A Weil[1]; James Pyke[2]; Michael Woodman[1]; Gosia Medrecki[3]; Melissa R Pergande[4]; *[1]Agilent Technologies, Wood Dale, IL; [2]Agilent Technologies, Santa Clara, CA; [3]Agilent Technologies, Wood Dale, IL; [4]University of Illinois at Chicago, Chicago, IL*

WP 535 **Overcoming Recovery Challenges in Hemolyzed Samples for the Determination of Propafenone and 5-Hydroxy Propafenone by LC-MS/MS**; Vinicio Vasquez[1]; Milton Furtado[1]; Mingluan Chen[1]; Anahita Keyhani[1]; *[1]Altasciences, Laval , QC*

WP 536 **Development and Validation of LC-MS/MS Method for Determining Temozolomide in Mouse Brain Following Intra-Cerebral Microdialysis**; Raghavi Kakarla[1]; Kimberly Yacoub[1]; Baochuan Guo[1]; *[1]Cleveland State University, Cleveland, OH*

WP 537 **Mass Spectrometry Based Analysis of Permethylated N-Glycans Purified and Separated using Microgradient Device**; Pavel Rehulka[1]; Martina Zahradnikova[2]; Lukas Uhrik[2]; Helena Rehulkova[1]; Rudolf Nenutil[2]; Lenka Hernychova[2]; Milos V. Novotny[3]; *[1]Faculty of Military Health Sci., Univ. of Defence, Hradec Kralove, Czech Republic; [2]Regional Centre for Applied Molecular Oncology, Masaryk Memorial Cancer Institute, Brno, Czech Republic; [3]Department of Chemistry, Indiana University, Bloomington, IN*

WP 538 **Automating Metabolic Stability Assays and Analyses using a Robotic Autosampler and LC/MS/MS Platform**; Fred D. Foster[1]; John R. Stuff[1]; Laurel A. Verarelli[1]; Jacqueline A. Whitecavage[1]; *[1]Gerstel, Inc., Linthicum, MD*

WP 539 **Comparison of SPE Protocols for Phospholipid Removal in Basic Analyte Bioanalytical Quantitation**; Melvin Blaze Muttikal Thomas[1]; Thomas H Walter[1]; Kenneth Berthelette[1]; Bonnie A Alden[1]; Donna Osterman[1]; Kevin Wyndham[1]; *[1]Waters Corporation, Milford, MA*

WP 540 **Cleanup of Pharmaceutical Drugs in Biological Fluids by Automated microSPE Prior to LC/MS**; Raquel Gonzalez de Vega[1]; Simin Maleknia[1]; Matthew Diplock[1]; Andrew Minett[2]; Philip Doble[1]; *[1]University of Technology Sydney, Sydney, Australia; [2]Eprep Pty Ltd, Mulgrave, Australia*

WP 541 **Blowing Analytical Precision and Accuracy out of the Water – microSPE of Explosives**; Matthew Diplock[1]; Raquel Gonzalez de Vega1[1]; Philip Doble[1]; Andrew Minett[2]; *[1]University of Technology Sydney, Sydney, Australia; [2]Eprep Pty Ltd, Mulgrave, Australia*

WP 542 **Fully Automated Determination of Phosphatidylethanol 16:0/18:1 and 16:0/18:2 in Dried Blood Spots**; Marc Joel Luginbuehl[1]; Stefan Gaugler[2]; Wolfgang Weinmann[1]; *[1]Institute of Forensic Medicine Bern, Bern, Switzerland; [2]CAMAG, Muttenz, Switzerland*

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WP 543 **Mechanism of Prostaglandin E2 Accumulation in Amniotic Fluid during Human Labor**; Toshiaki Okuno[1]; Nanase Takahashi[1]; Takehiko Yokomizo[1]; *[1]Department of Biochemistry, Juntendo University School of Medicine, Tokyo, Japan*

WP 544 **Screening New Reagents for the Paternò-Büchi Reactions for Lipid Analysis by Mass Spectrometry**; Jing Zhao[1]; Xiaobo Xie[1]; Yu Xia[1]; *[1]Tsinghua University, Beijing, China*

WP 545 **Investigating Enzymatic Lipase Activity via Contained-Electrospray Ionization (ESI) Mass Spectrometry as a Function of Secondary Organic Aerosol (SOA) Evolution**; Mickey M. Rogers[1]; Benjamin J. Burris[1]; Abraham K. Badu-Tawiah[1]; *[1]The Ohio State University, Columbus, OH*

WP 546 **Top-Down Shotgun Lipidomics Analysis with Ultra-High Resolution Orbitrap Mass Spectrometry**; Kai Schuhmann[1]; Konstantin Nagornov[2]; Anton Kozhinov[2]; Yury Tsybin[2]; Andrej Shevchenko[1]; *[1]MPI-CBG, Dresden, Germany; [2]Spectroswiss Sàrl, Lausanne, Switzerland*

WP 547 **Quantitative Analysis of Trans-Fatty Acids in Humans**; Heather C Kuiper[1]; Na Wei[1]; Emily J Mueller[1]; Sarah W Kingsley[1]; Hubert W Vesper[1]; *[1]CDC, Atlanta, GA*

WP 548 **Analysis of Oxidized Cardiolipins by Solid Phase Extraction and LC/MS**; Gaoyuan Liu[1]; Richard W Gross[2]; *[1]Washington University in Saint Louis, Saint Louis, MO; [2]Washington University School of Medicine, St. Louis, MO*

WP 549 **Acute-phase Serum Lipidome Alterations in a Rodent Model of Closed Head Traumatic Brain Injury**; Scott Hogan[1]; Kyle Milligan[2]; Michelle LaPlaca[2]; Facundo M Fernandez[1]; *[1]Georgia Institute of Technology, School of Chemistry and Biochemistry, Atlanta, Georgia; [2]Georgia Institute of Technology, Department of Biomedical Engineering, Atlanta, Georgia*

WP 550 **Comparative Analysis of Nutritional Lipids from Marine Sources by Supercritical Fluid Chromatography with Tandem Mass Spectrometry**; Greg Winter[1]; Paolo Lecchi[1]; Craig Mallon[1]; Dominik Burger[1]; *[1]DSM, Columbia, MD*

WP 551 **Serum Lipidomics of Pregnant African American Women Exposed to Environmental Toxicants**; Anna A Ivanova[1]; Kristal Maner-Smith[1]; Dana Boyd Barr[1]; Anne L Dunlop[1]; Eric A Ortlund[1]; *[1]Emory University, Atlanta, GA*

WP 552 **Analysis of Very Long Chain Fatty Acids by Supercritical Fluid Chromatography-Mass Spectrometry**; Paolo Lecchi[1]; Gregory Winter[1]; Dominik Burger[1]; Srujana Beeram[1]; *[1]DSM Nutritional Products, Columbia, MD*

WP 553 **Triglyceride Precursor Pool Enrichment and *de novo* Lipogenesis in Plasma Lipoproteins Probed by Stable-Isotope GC/MS-MIDA Methodology Using Multiple Tracer-Administration Protocols**; Sergiu P. Palii[1]; Grace M. Jones[1]; Mariel Dologmandin[1]; Zachary Woodward[1]; David Doud[1]; Jean-Marc Schwarz[1,2]; *[1]Touro University California, Vallejo, CA; [2]University of California, San Francisco (UCSF), San Francisco, CA*

WP 554 **Discovery of Novel LPA-Binding Proteins Using a Chemical Proteomic Method**; Xuejiao Dong[1]; Yinsheng Wang[1]; *[1]UC Riverside, Riverside*

WP 555 **Effect of Matrix Type and Storage Conditions on Lipid Profiles of Clinical Blood Samples**; Rahul Deshpande[1]; Kaitlyn Scola[1]; Tim Wood[1]; *[1]Greenwood Genetic Center, Greenwood, SC*

WP 556 **Lipid profiling of Chromochloris zofingiensisin Photoautotrophic and Heterotrophic Cultures**; Yuntao Hu[1,2]; Melissa S Roth[2]; Katherine Louie[1,3]; Benjamin Bowen[1,3]; Krishna Niyogi[2]; Trent Northen[1,3]; *[1]Lawrence Berkeley Laboratory, Berkeley, CA; [2]University of California, Berkley, Berkeley, CA; [3]Joint Genome Institute, Walnut Creek, CA*

WP 557 **Lipidomic Analyses of Wild Type, Knock-Out, S508D-, and S508A-CEACAM1 Heptocarcinoma Cells;** Gabriel B Gugiu[1,2,3]; Jennifer Chean[1,2]; Charng Chen[1,2]; John E Shively[1,2]; *[1]City of Hope, Duarte, CA; [2]Beckman Research Institute, Department of Molecular Imaging and Therapy, Duarte, CA; [3]Beckman Research Institute, Department of Shared Resources, Mass Spectrometry and Proteomics Core Facility, Duarte, CA*

WP 558 **High Speed Untargeted Lipidomics and Metabolomics LC-MS/MS workflows with Parallel Accumulation Serial Fragmentation (PASEF);** Ulrike Schweiger-Hufnagel[1]; Aiko Barsch[1]; Sven W. Meyer[1]; *[1]Bruker Daltonics, Bremen, Germany*

WP 559 **The Regulation of the Molecular Structural Diversity of Mitochondrial Cardiolipins in Mouse Tissues;** Gregor Oemer[1]; Jakob Koch[2]; Mohammed Tauqeer Alam[3]; Marie-Luise Edenhofer[2]; Sabrina Sailer[4]; Carolina Doerrier[5]; Ernst R Werner[4]; Katrin Watschinger[4]; Erich Gnaiger[5]; Johannes Zschocke[2]; Markus A Keller[2]; *[1]Division of Human Genetics, Medical Unversity of Innsbruck, Innsbruck, Austria; [2]Division of Human Genetics, Medical Unversity of Innsbruck, Innsbruck, Austria; [3]Division of Biomedical Sciences, Warwick Medical School, University of Warwick, Warwick, United Kingdom; [4]Division of Biological Chemistry, Biocenter, Medical University of Innsbruck, Innsbruck, Austria; [5]Oroboros Instruments Corporation, Innsbruck, Austria*

WP 560 **Fatty Liver is More than Neutral Lipid Accumulation: An Analysis of Human Non-Alcoholic Fatty Liver by Shotgun Lipidomics;** Olga Vvedenskaya[1]; Oskar Knittelfelder[1]; Eduardo Jacobo Miranda Ackerman[1]; Josch Pauling[2]; Judith Wodke[3]; Jochen Hampe[4]; Andrej Shevchenko[5]; *[1]Max Planck Institute of Molecular Cell Biology and Genetics, Dresden, Germany; [2]Technische Universität München, Freising, Germany; [3]Humboldt University, Berlin, Germany; [4]Dresden University Clinic, Dresden, Germany; [5]Max Plank Institute for Molecular Cell Biology and Genetics, Dresden, Germany*

WP 561 **Mass Spectrometric Study on the Source of Error in Quantification of Free Fatty Acids;** Hyejin Park[1]; Tae-Young Kim[1]; *[1]School of Earth Sciences and Environmental Engineering, Gwangju Institute of Science and Technology, Gwangju, South Korea*

WP 562 **Trapped Ion Mobility Spectrometry (TIMS) and Parallel Accumulation Serial Fragmentation (PASEF) for Nanoflow LC-MS/MS-Based Lipidomics;** Catherine G. Vasilopoulou[1]; Karolina Sulek[2]; Andreas-David Brunner[1]; Sven W. Meyer[3]; Ulrike Schweiger-Hufnagel[3]; Ningombam Sanjib Meitei[4]; Matthias Mann[1,2]; Florian Meier[1]; *[1]Max Planck Institute of Biochemistry, Martinsried, Germany; [2]NNF Center for Protein Research University of Copenhagen, Copenhagen, Denmark; [3]Bruker Daltonik GmbH, Bremen, Germany; [4]PREMIER Biosoft, Palo Alto, CA*

WP 563 **Lipidomics of Dolphin Serum to Assess Physiological and Ecological Changes Following the Deepwater Horizon Oil Spill;** Michael P. Napolitano[1,2]; Maggie Broadwater[1]; Tracey B. Schock[2,3]; Ryan Takeshita[4]; Terri K. Rowles[5]; Lori H. Schwacke[6]; *[1]National Oceanic and Atmospheric Administration, Charleston, SC; [2]Hollings Marine Laboratory, Charleston, SC; [3]National Institute of Standards and Technology, Charleston, SC; [4]National Marine Mammal Foundation, Boulder, CO; [5]National Oceanic and Atmospheric Administration, Silver Spring, MD; [6]National Marine Mammal Foundation, Charleston, SC*

WP 564 **Sample Preparation Effects on Retinal Lipid Analysis by MALDI Imaging and LC-MS Technologies;** Ankita Kotnala; *Vanderbilt University, Nashville, TN*

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WP 565 **MxP® Quant 500 Kit – Novel Standardized Metabolomics/Lipidomics Analysis Tool for Comprehensive Targeted Profiling;** Hai Pham Tuan[1]; Ulf Sommer[1]; Svenja Heischmann[1]; Doreen Kirchberg[1]; Xenia Iwanowa[1]; Radu Talmazan[1]; Barbara Wolf[1]; Martin Buratti[1]; Rosa Arganasilla Martinez[1]; Cornelia Röhring[1]; Therese Koal[1]; *[1]BIOCRATES Life Sciences AG, Innsbruck, Austria*

WP 566 **New Features and Functions of the Old "Mustard Oil Bomb" in Single Cell-Types;** Shweta Chhajed[1]; Craig Dufresne[2]; Nathalia Tello[1,3]; Alice Harmon[1,4,5]; Sixue Chen[1,4,5,6]; *[1]Department of Biology, University of Florida, Gainesville, FL; [2]Thermo Fisher Scientific, West Palm Beach, FL; [3]SF2UF Bridge Program, University of Florida, Gainesville, FL; [4]Plant Molecular and Cellular Biology, University of Florida, Gainesville, FL; [5]Genetics Institute, University of Florida, Gainesville, FL; [6]nterdisciplinary Center for Biotechnology Research, University of Florida, Gainesville, FL*

WP 567 **Effects of Acute Ambient PM2.5 Exposure on Heart in C57BL/6J Diet-Induced Obesity Mouse Model;** Yuanyuan Song[1]; Yanhao Zhang[1]; Zenghua Qi[2]; Ruijin Li[3]; Zongwei Cai[1]; *[1]Hong Kong Baptist University, Hong Kong, China; [2]Guangdong University of Technology, Guangzhou, China; [3]Shanxi University, Taiyuan, China*

WP 568 **Meta-Analysis of Targeted Metabolomics Data from Heterogeneous Biological Samples Provides Insights into Metabolite Dynamics;** Ho-Joon Lee[1]; Daniel Kremer[1]; Peter Sajjakulnukit[1]; Li Zhang[1]; Costas Lyssiotis[1]; *[1]University of Michigan Medical School, Ann Arbor, MI*

WP 569 **Targeted Multi-OMICS: Rapid Plasma Profiling of a Bladder and Lung Cancer Human Cohort;** Sarah Lennon[1]; Billy J Molloy[1]; Lee A Gethings[1]; Robert S Plumb[2]; Andrew Peck[2]; *[1]Waters corporation, Wilmslow, United Kingdom; [2]Waters Corporation, Milford, MA*

WP 570 **An Improved Isotope-Labeling Chemical Derivatization – LC/MRM-MS Method for Reliable Quantitation of >70 FAs in Human Serum;** Jun Han[1,2]; Kieran Atkinson[1]; Evan Dyson-Loewen[1]; Mia Frier[1]; Juncong Yang[1]; John Ducas[3]; Robin Ducas[3]; Erin Weldon[4]; Tom Jelic[4]; R. Antony Shaw[5]; Christoph H. Borchers[1,6,7,8]; *[1]University of Victoria-Genome BC Proteomics Centre, Victoria, BC; [2]Division of Medical Sciences, University of Victoria, Victoria, BC; [3]Faculty of Medicine, Department of Cardiology, University of Manitoba, Winnipeg, Manitoba; [4]Faculty of Medicine, Department of Emergency Medicine, University of Manitoba, Winnipeg, Manitoba; [5]National Research Council of Canada, Winnipeg, Manitoba; [6]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; [7]Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; [8]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC*

WP 571 **Quantification of Polar Metabolites in Urine using an Automated Parallel Derivatization Strategy andLC-SWATH-MS;** Guenter Boehm[1]; Maria Fernanda Cifuentes Girard[2]; David Ruscic[3]; Renzo Picenoni[1]; Gerard Hopfgartner[3]; *[1]CTC Analytics AG, Zwingen, Switzerland; [2]Life Sciences Mass Spectrometry, Department of analytical and Inorganic Chemistry, University of Geneva, Geneva, Switzerland; [3]Life Sciences Mass Spectrometry, Department of analytical and Inorganic Chemistry, University of Geneva, Geneva, Switzerland*

WP 572 **Isotope-Labeled Metabolic Flux Analysis of the Gut Microbiota-Driven Carnitine Metabolism;** Hsin-bai Zou[1]; Fang-Wei Kuo[2]; Qiang Lyu[3]; Hsin-Yuan Chang[3]; Cheng-Chih Hsu[3]; Wei-Kai Wu[4]; *[1]Department of Chemistry, National Taiwan University, taipei, Taiwan; [2]Institute of*

food science and technology, taipei, Taiwan; [3]Department of Chemistry, National Taiwan University, Taipei, Taiwan; [4]Department of Internal Medicine, National Taiwan University Hospital Bei-Hu Branch, Taipei, Taiwan, taipei, Taiwan

WP 573 **Multiplexed High Throughput LC-MS/MS Method for Targeted Metabolites and Neurotransmitters from Central Nervous System;** Juho Heininen[1]; Tapio Kotiaho[1]; Anu Vaikkinen[1]; Risto Kostiainen[1]; *[1]University of Helsinki, Helsinki, Finland*

WP 574 **Derivatisation of Central Metabolites in SUIT-2 Cells Using 2-bromo-1-(4-dimethylamino-phenyl)-ethanone Enables LC-MS/MS Energy-State Analysis;** Cornelius C W Willacey[1]; Martijn Naaktgeboren[1]; Edinson Lucumi Moreno[1]; Alida S D Kindt[1]; Daan van der Es[2]; Ronan M T Fleming[1]; Amy C Harms[1]; Thomas Hankemeier[1]; *[1]Analytical BioSciences and Metabolomics, Systems Biomedicine and Pharmacology, Leiden Academic Centre for Drug Research, Leiden University, Leiden, Netherlands; [2]Medicinal Chemistry, Drug Discovery and Safety, Leiden Academic Centre for Drug Research, Leiden University, Leiden, The Netherlands, Leiden, Netherlands*

WP 575 **Assessment of the Microbiota Metabolome and Its Role in Cardiovascular Diseases;** Tuan Hai Pham[1]; Ulf Sommer[1]; Svenja Heischmann[1]; Barbara Wolf[1]; Fadi Abdi[1]; Therese Koal[1]; *[1]BIOCRATES Life Sciences AG, Innsbruck, Austria*

WP 576 **Quantitative Comparison of the Suppression between HILIC and Reverse Phase Chromatography;** Lucas Veillon[1]; John N Weinstein[1]; Phil Lorenzi[1]; Felice A de Jong[2]; Chris Beecher[2]; *[1]MD Anderson Cancer Center, Houston, TX; [2]IROA Technologies LLC, Bolton, MA*

WP 577 **5-plex iDiLeu Enabled Neurotransmitter Absolute Quantitation in the Crustacean Nervous System;** Qinjingwen Cao[1]; Gongyu Li[1]; Amanda R. Buchberger[1]; Lingjun Li[1]; *[1]University of Wisconsin-Madison, Madison, WI*

WP 578 **Rapid Automated Absolute Quantification of Metabolites Using Polly QuantFit to Understand Tumor Nutrient Availability;** Abhishek Jha[1]; Avijit Zutishi[2]; Raghav Sehgal[2]; Shubham Agarwal[2]; Taranjyot Singh[2]; Shefali Lathwal[2]; Swetabh Pathak[2]; Alex Muir[3]; Caroline Lewis[4]; Mark Sullivan[3]; Matthew G. Vander Heiden[3]; *[1]Elucidata, Cambridge, MA; [2]Elucidata, Delhi, India; [3]Massachusetts Institute of Technology, Cambridge, MA; [4]Whitehead Intitute, Cambridge, MA*

WP 579 **Simultaneous Analysis of Steroids and Lipids in Serum Employing Liquid Chromatography-Ion Mobility Spectrometry-Mass Spectrometry Analysis;** Alana Rister[1]; Katie L Bidne[1]; Jennifer R Wood[1]; Eric D. Dodds[1]; *[1]University of Nebraska - Lincoln, Lincoln, NE*

WP 580 **Direct Quantification of Polyamines in Arabidopsis thaliana seedlings by LC-MS/MS;** Masoud Zabet Moghaddam[1]; parvin mirzaei[2]; mohamed Fokar[2]; Yehia Mechref[3]; *[1]Texas Tech University, Box 43132 Lubbock, TX; [2]Texas Tech University, Lubbock, TX; [3]Texas Tech University, Lubbock*

WP 581 **Innovative One-Step Protocol for Producing Deuterium-Labeled Metabolites and Their Use for Quantitative LC-HRMS-Based Targeted Metabolomics;** Annelaure Damont[1]; Yu Min Kiw[1]; Kathleen Rousseau[1]; Sophie Feuillastre[2]; Grégory Pieters[2]; Christophe Junot[3]; François Fenaille[1]; *[1]Service de Pharmacologie et Immunoanalyse (SPI), Laboratoire d'Etude du Métabolisme des Médicaments (LEMM), CEA, INRA, Université Paris-Saclay, MetaboHUB-IDF, Gif-Sur-Yvette, France; [2]Service de Chimie Bio-organique et de Marquage, Laboratoire de Marquage au Tritium, Département Médicaments et Technologies pour la Santé, Institut Joliot, CEA, Université Paris-Saclay, Gif-Sur-Yvette, France; [3]Service de Pharmacologie et Immunoanalyse (SPI), Département Médicaments et Technologies pour la Santé, Institut Joliot, CEA, INRA, Université Paris-Saclay, MetaboHUB-IDF, Gif-Sur-Yvette, France*

WP 582 **Reovirus-Induced Alterations in the Metabolome of M1 and M2 Macrophages;** Michael Giacomantonio[1]; Patrick J Murphy[1]; Barry Kennedy[1]; Shashi Gujar[1, 2]; *[1]Department of Pathology, Dalhousie University, Halifax, NS, Canada, Halifax, NS; [2]Department of Microbiology and Immunology, Dalhousie University, Halifax, NS, Canada, Halifax, NS, Canada, Halifax, NS*

WP 583 **Profiling of Bile Acids, Histidine, and Histamine in Gastric Juice by LC-MS/MS Combined with Serial Derivatization: Diagnosis of Gastric Cancer;** Wonwoong Lee[1]; Jinhee Um[1]; Keon-hee Ko[1]; Bong Chul Chung[2]; Jongki Hong[1]; *[1]Kyung Hee University, Seoul, South Korea; [2]Korea Institute of Science and Technology, Seoul, South Korea*

WP 584 **Rapid LC-MS/MS Method for Targeted Quantitation of Human Performance Metabolites in Saliva;** Ethan M McBride[1]; Richard J Lawrence[1]; Kirstin McGee[1]; Phillip M Mach[1]; Paul S Demond[2]; Michael W Busch[2]; John W Ramsay[3]; Erika K Hussey[3]; Trevor Glaros[1]; Elizabeth S Dhummakupt[1]; *[1]Research and Technology Directorate, Research Development & Engineering Command (RDECOM) Edgewood Chemical Biological Center (ECBC), Aberdeen Proving Ground, MD; [2]Excet, Inc., Springfield, VA; [3]U.S. Army Natick Soldier Research, Development & Engineering Center, Natick, MA*

WP 585 **Spatial Distribution of Ractopamine Residues in Bovine muscle;** Valerie Lindstrom[1]; Haley E Davis[1]; Jacqueline M Chaparro[1]; Keith E Belk[1]; Jessica E. Prenni[1]; *[1]Colorado State University, Fort Collins, CO*

WP 586 **Improving the Accuracy of Endogenous tZ-Type Cytokinins Determination by Elucidation of the Fragmentation Mechanism;** Peiyong Xin[1]; Jinfang Chu[1]; *[1]National Center for Plant Gene Research (Beijing), Institute of Genetics and Developmental Biology, Chinese Academy of Sciences, Beijing, China*

WP 587 **Measurement of Metabolites in Feces of Japanese Rock Ptarmigans by LC-MS/MS;** Takanari Hattori[1]; Yukari Oka[1]; Shuichi Kawana[1]; Koretsugu Ogata[1]; Sayaka Tsuchida[2, 3]; Atsushi Kobayashi[4]; Yoshiaki Nakamura[5]; Hiroshi Nakamura[6]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Kyoto Prefectural University, Kyoto, Japan; [3]Chubu University, Kasugai, Japan; [4]Toho University, Tokyo, Japan; [5]Hiroshima University, Hiroshima, Japan; [6]Nakamura Hiroshi International Institute for Ornithology, Nagano, Japan*

WP 588 **Rapid Throughput Quantitation of Carboxylic Acid Metabolites Using UHPLC/QqQ-MS to Monitor Diet and the Microbiome;** Diane Tu[1]; Carol Stroble[1]; Matthew J. Amicucci[1]; Gege Xu[1]; Jennifer T Smilowitz[1]; Carlito B Lebrilla[1]; *[1]University of California, Davis, Davis, CA*

WP 589 **A Critical Look at Highly Mulitplexed Targeted Metabolomics: Data Quality Effects from Large Target Lists;** Robert Pepin[1]; Mathew Ellenberger[1]; Daniel Raftery[1, 2]; *[1]University of Washington, Seattle, WA; [2]Fred Hutchinson Cancer Research Center, Seattle, WA*

WP 590 **Simultaneous Detection of Tricarboxylic Acid Cycle Intermediates using LC-MS/MS with a Synergi® Fusion-RP HPLC Column;** Xianrong (Jenny) Wei[1]; Ryan Splitstone[1]; Sean Orlowicz[1]; *[1]Phenomenex, Torrance, CA*

WP 591 **Comparative Metabolomics of *Staphylococcus aureus* by HPLC-DAD-MS/MS;** Gerson D. López[1]; Chad Leidy[1]; Chiara Carazzone[1]; *[1]Universidad de los Andes, Bogotá D.C, Colombia*

WP 592 **Development of a UPLC-MS/MS Method to Quantitate Process-Induced Nitrogen Compounds and their Metabolites in Urine Samples;** Yi-Chen Sun[1]; Hsin-Chang Chen[1]; *[1]Institute of Food Safety and Health, National Taiwan University, Taipei, Taiwan*

WP 593 **Analysis of Endogenous Steroid Hormones in Urine Using High-Resolution LC-MS**; Lancia N.F. Darville-bowleg[1]; Min Liu[1]; Jayden Cline[1]; Yessica C. Martinez-Monta[1]; Shannan Rich[2]; John Koomen[1]; Lusine Yaghjyan[2]; Kathleen M Egan[1]; *[1]Moffitt Cancer Center, Tampa, FL; [2]University of Florida, Gainesville, FL*

WP 594 **Gut Microbial and Hepatic Metabolism of the Hop Flavonoid, Xanthohumol, in Humans**; Wenbin Wu[1]; Ines L Paraiso[1]; Ralph Reed[1]; Jeffrey Morré[2]; Jan F. Stevens[1]; *[1]Department of Pharmaceutical Sciences, Linus Pauling Institute, Oregon State University, Corvallis, Oregon; [2]Department of Chemistry, Oregon State University, Corvallis, Oregon*

WP 595 **Fit-for-Purpose Quantitative LC-MS and CE-MS Metabolomics Methods to Inform Alzheimer's Research**; Kendra J. Adams[1]; J. Will Thompson[1]; W. Kirby Gottschalk[1]; Joan G. Wilson[1]; M. Arthur Moseley[1]; Carol A. Colton[1]; *[1]Duke University School of Medicine, Durham, NC*

WP 596 **A Novel and Comprehensive Steroid Assay Including Thyroxin Compounds Using Small Volume Human Serum or Plasma Samples**; Gregory Byram[1]; Chris Vanselow[2]; Patrick Fitzgerald[1]; Catherine Paige Riley[3]; Stacy Tremintin[2]; Oliver Fiehn[1]; *[1]UC Davis West Coast Metabolomics Center, Davis, CA; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, West Palm Beach, FL*

WP 597 **Probing the Altered Microbiome of ASD for Metabolic Clues**; Emily R. Sekera[1]; Troy D. Wood[1]; Heather L. Rudolph[1]; *[1]University at Buffalo, Buffalo, NY*

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WP 598 **Untargeted Metabolomics Profiling of Longitudinal Urine Samples Collected from Individual Participant of Integrated Personalized Omics Profiling (iPOP) Project**; Songjie Chen[1]; Liang Liang[1]; Yuqin Dai[2]; Michael Snyder[1]; *[1]Stanford University, Stanford, CA; [2]Agilent, Santa Clara, CA*

WP 599 **Using Mass Spectrometry-Based Metabolomics to Explore Polyphenol Profile Diversity among Different Lentil Seed Coat Colors and Patterns**; Fatma M. Elessawy[1]; Derek Wright[1]; Albert Vandenberg[1]; Anas El-Aneed[1]; Randall W. Purves[1,2]; *[1]University of Saskatchewan, Saskatoon, SK; [2]Canadian Food Inspection Agency, Saskatoon, SK*

WP 600 **Correcting Metabolomic Data for Source Variances Using IROA**; Fei Tang[1]; Felice de Jong[2]; Chris Beecher[2]; Markos Leggas[1]; *[1]University of Kentucky, Lexington, KY; [2]IROA Technologies LLC, Bolton, MA*

WP 601 **Untargeted Profiling of Metabolites, Nutrients, and Toxins in Sera from the Isle of Wight Multigenerational Birth Cohort**; Thilani M. Anthony[1]; Wilfried J. J. Karmaus[2]; Su Chen[3]; Susan Ewart[4]; Syed Hasan Arshad[5,6,7]; John W. Holloway[6]; Hongmei Zhang[2]; A. Daniel Jones[1,9]; *[1]Department of Biochemistry & Molecular Biology, Michigan State University, East Lansing, MI; [2]Division of Epidemiology, Biostatistics, and Environmental Health, School of Public Health, University of Memphis, Memphis, Tennessee; [3]Department of Mathematical Sciences, University of Memphis, Memphis, Tennessee; [4]Department of Large Animal Clinical Sciences, College of Veterinary Medicine, Michigan State University, East Lansing, MI; [5]Clinical and Experimental Sciences, Faculty of Medicine, University of Southampton, Southampton, United Kingdom; [6]The David Hide Asthma and Allergy Research Centre, Isle of Wight, United Kingdom; [7]NIHR Respiratory Biomedical Research Unit, University Hospital Southampton, Southampton, United Kingdom; [8]Human Development and Health, University of Southampton, Southampton, United Kingdom; [9]Department of Chemistry, Michigan State University, East Lansing, MI*

WP 602 **A Metabolomics Study into during Infection with Influenza Virus by HRAM Q-TOF Analysis**; Emily Armitage[1]; Jonathan Swann[2]; Mick Bailey[3]; Ian D Wilson[2]; Neil J Loftus[1]; *[1]Shimadzu MS/BU, Manchester, United Kingdom; [2]Imperial College London, Department of Surgery and Cancer, United Kingdom; [3]School of Veterinary Sciences, University of Bristol, Bristol, United Kingdom*

WP 603 **Using IROA-Based Internal Standard Normalization to Minimize Non-IROA Metabolite Variation**; Chris Beecher[1]; Felice de Jong[2]; *[1]IROA Technologies, Chapel Hill, NC; [2]IROA Technologies LLC, Bolton, MA*

WP 604 **Regaining the ASHES: Finding Chemical 'Clues' to Mitigate the Impact OF Ash Dieback**; John D Sidda[1]; Christine M Sambles[2]; Lijiang Song[1]; Murray R Grant[1]; *[1]University of Warwick, Coventry, United Kingdom; [2]University of Exeter, Exeter, United Kingdom*

WP 605 **Proteometabolomics of Bortezomib Resistance in Multiple Myeloma**; David C. Koomen[1]; Joy D. Guingab-Cagmat[2]; Paula S. Oliveira[1]; Bin Fang[1]; Min Liu[1]; Eric A. Welsh[1]; Mark B. Meads[1]; Tuan Nguyen[1]; Laurel E. Meke[2]; Steven A. Eschrich[1]; Timothy J. Garrett[2]; John M. Koomen[1]; Kenneth H. Shain[1]; *[1]H. Lee Moffitt Cancer Center, Tampa, FL; [2]University of Florida, Gainesville, FL*

WP 606 **Untargeted Metabolomics of Bumble Bee Cold Tolerance Using Stacked Injection of Biphasic Extraction with LC-MS/MS**; Mitchell Helling[1]; Kennan J. Oyen[1]; Michael E. Dillon[1]; Franco Basile[1]; *[1]University of Wyoming, Laramie, WY*

WP 607 **Methanol Quenching Versus Flash Freezing for Metabolomics Profiling of Wheat Leaves**; Marie J. Andales[1]; Linxing Yao[2]; Corey D. Broeckling[1]; Kaitlyn Maloley[1]; *[1]Proteomics & Metabolomics Facility, Colorado State University, Fort Collins, CO; [2]Proteomics and Metabolomics Facility of Colorado State University, Fort Collins, CO*

WP 608 **A Metabolomic SWATH-MS Approach Applied to PBMCs from First Psychotic Episode Patients**; Margarida Coelho[1]; Vera M Mendes[1]; Cátia Santa[1]; Manuel Coroa[2]; Sofia Morais[2]; Inês Baldeiras[1]; Nuno Madeira[2]; Antonio Macedo[2]; Bruno Manadas[1]; *[1]Center for Neuroscience and Cell Biology, Cantanhede, Portugal; [2]Psychiatry department, CHUC, Coimbra, Portugal*

WP 609 **Development and Application of a Novel Metabolomics Platform Based on Capillary Electrophoresis Coupled with a High-Resolution Mass Spectrometry**; Kazunori Sasaki[1]; Hitoshi Sagawa[1]; Makoto Suzuki[1]; Kaori Abe[1]; Satoshi Ito[2]; Tsutomu Negama[2]; Moon-Il Kang[1]; Kenjiro Kami[1]; *[1]Human Metabolome Technologies, Tsuruoka, Japan; [2]Sekisui Medical Company, Chuo-ku, Japan*

WP 610 **Comparison of Data-Dependent Acquisition Methods on an Orbitrap ID-X**; Kevin Y Cho[1]; Fuad J Naser[1]; Michaela Schwaiger-Haber[1]; Miriam Sindelar[1]; Gary J Patti[1]; *[1]Washington University in St. Louis, St. Louis, MO*

WP 611 **A Systematic Approach to Development of Analytical Scale and Microflow-based LC-MS Metabolomics Methods to Support Drug Discovery and Development**; Sarah Geller[1]; Harvey Lieberman[1]; Alla Kloss[1]; Alexander R Ivanov[2]; *[1]Sanofi, Waltham, MA; [2]Department of Chemistry and Chemical Biology, Northeastern University, Boston, MA*

WP 612 **Metabolomics Analysis of Respirofermentative Phenotypes in a Crabtree-Positive and -Negative Yeast**; April Miguez[1]; Mark Styczynski[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

WP 613 **Separation and Analysis of Low Molecular Weight Organic Acid Metabolites by Mixed-Mode Chromatography Coupled to Mass Spectrometry**; Kerri Smith[1]; Paul D Rainville[1]; *[1]Waters Corporation, Milford, MA*

WP 614 **Quantitative Metabolomics, Histology and Clinical Pathology Using the Exact Same Tissue Sample: Two-for-One Analyses for Biomarker Discovery**; Dorothea Y. Mung[1]; Stephen L. Carrithers[2]; Richard T. Coughlin[2]; Dean A. Troyer[3]; Liang Li[4]; *[1]Nova Medical Testing Inc., Edmonton, AB; [2]Lagrange Scientific LLC, Pewee Valley, KY; [3]Eastern Virginia Medical School, Norfolk, VA; [4]University of Alberta, Edmonton, AB*

WP 615 **MDM2 Copy Number Aberrations Alter Ceramide Glycosylation in Liposarcoma Tumors, Impacting Drug Response**; Andrew Patt[1]; Bryce Demorel[1]; Andrew Patterson[2]; Philip Smith[2]; Ewy Mathe[1]; James Chen[1]; *[1]The Ohio State University, Columbus, OH; [2]Pennsylvania State University, State College, PA*

WP 616 **Analysis of Volatile Organic Profiles in Stem Cells by Comprehensive Two-Dimensional Gas Chromatography with Time-of-Flight Mass Spectrometry**; Christopher A. Heist[1]; Jean-marie D. Dimandja[2]; Milad Navaei[1]; *[1]Georgia Tech Research Institute, Atlanta, GA; [2]Georgia Institute of Technology, Department of Mechanical Engineering, Atlanta, GA*

WP 617 **Stable Isotope Label-Supported IM-QRAI Methods for Metabolomics**; Max Feuerstein[1]; Ruwan T. Kurulugama[2]; John C. Fjeldsted[2]; Tim Causon[1]; Stephan Hann[1]; *[1]Institute of Analytical Chemistry, Department of Chemistry, University of Natural Resources and Life Sciences (BOKU), Vienna, Austria; [2]Agilent Technologies, Inc., Santa Clara, CA*

WP 618 **Integrating 4D Peak Picking of LC-TIMS-MS/MS Data into GNPS Feature Based Molecular Networking for Metabolomics and Lipidomics Analysis**; Florian Zubeil[1]; Nikolas Kessler[1]; Heiko Neuweger[1]; Sven W. Meyer[1]; Ulrike Schweiger-Hufnagel[1]; Aiko Barsch[1]; *[1]Bruker Daltonik GmbH, Bremen, Germany*

WP 619 **Robust and Sensitive Untargeted Microflow Metabolomics with OptiFlow™ Turbo V Source**; Khatereh Motamedchaboki[1]; Carmai Carmai[2]; Lekha Sleno[3]; Vivaldy Prinville[3]; *[1]Sciex, Redwood City, CA; [2]SCIEX, Concord, ON; [3]Universite du Quebec a Montreal, Montreal, Québec*

WP 620 **Development of 4-Channel Chemical Isotope Labeling LC-MS for Comprehensive Profiling of the Human Tear Metabolome**; Kevin Hooton[1]; Gavin SW Tan[2,3,4,5]; Lei Zhou[2,4,5]; Liang Li[6]; *[1]Nova Medical Testing Inc., Edmonton, AB; [2]Singapore Eye Research Institute, Singapore, Singapore; [3]Singapore National Eye Center, Singapore, Singapore; [4]Duke-NUS Medical School, Singapore, Singapore; [5]National University of Singapore, Singapore, Singapore; [6]University of Alberta, Edmonton, AB*

WP 621 **HILIC-HR-MS for (untargeted) Metabolomics in Microorganisms – the Optimal Method for Polar Compounds in an Industrial Setting?**; Leon Coulier[1]; Wouter Coppes[1]; Raymond Ramaker[1]; Sandra Pous-Torres[1]; *[1]DSM Biotechnology Center, Delft, Netherlands*

WP 622 **Nutrient Addition Effect on Four Setaria Accessions in Marginal Soil: Deciphering Plant-Ectorhizosphere's Relationships under Nutrient Limitation**; Matthew J Peterson[1]; Pubudu P. Handakumbura[1]; Zachary R. Russell[1]; Christer Jansson[1]; Young-Mo Kim[1]; Sarah J. Fansler[1]; Montana L. Smith[1]; Jason G. Toyoda[1]; Rosalie K. Chu[1]; Bryan A. Stanfill[1]; Steven C. Fransen[2]; Kim K. Hixson[1]; Stephen J. Callister[1]; *[1]Pacific Northwest National Laboratory, Richland, WA; [2]Washington State University Irrigation Agriculture Research and Extension Center, Prosser, WA*

WP 623 **Unifying Ionization Efficiencies: Quantitative Comparison of Diverse Data Sets and Validation of Prediction Models**; Piia Liigand[1]; Jaanus Liigand[1]; Karl Kaupmees[1]; Anneli Kruve[1]; *[1]University of Tartu, Institute of Chemistry, Tartu, Estonia*

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WP 624 **Investigation of the Formation and Structure Characteristics of miR-92a G-quadruplex by ESI-MS**; Min Xi[1,2]; Jiang Zhou[1]; Yizhou Li[2]; *[1]College of Chemistry and Molecular Engineering, Peking University, Beijing, China; [2]School of Pharmaceutical Sciences, Chongqing University, Shapingba, China*

WP 625 **Nucleotide Composition Analysis of Unknown Synthetic Oligo Products**; Roger G Moore[1]; Denise A Keen[1]; Piotr Swiderski[1]; Marcin Kortylewski[1]; Markus Kalkum[1]; *[1]City of Hope, Duarte, CA*

WP 626 **Compliant-Ready Workflow for Mass Confirmation Of Oligonucleotide and Related Impurities**; Andrew Tudor[1]; Maria Basanta-sanchez[2]; Alessio Zammataro[3]; Barry Dyson[3]; Laetitia Denbigh[3]; *[1]waters, Wilmslow, United Kingdom; [2]Waters Corporation, Pleasanton, CA; [3]Waters Corporation, Wilmslow, United Kingdom*

WP 627 **Binding of Phenanthroline-Neomycin Conjugates with Different G-Quadruplex DNA Investigated by ESI Mass Spectrometry and Isothermal Titration Calorimetry**; Mandeep Singh[1]; Vanessa Marie Rangel[1]; Ryan Hekman[1]; Craig Vierra[1]; Liang Xue[1]; *[1]University of the Pacific, Stockton, CA*

WP 628 **DNA/RNA Adducts Formation from Bisphenol F 3,4-Quinone Metabolite**; Wang Xiaoxiao[1]; Zhao Hongzhi[2]; Cai Zongwei[2]; *[1]State Key Laboratory of Environmental and Biological Analysis, Department of Chemistry, Hong Kong Baptist University, Hong Kong, China; [2]State Key Laboratory of Environmental and Biological Analysis, Department of Chemistry, Hong Kong Baptist University, HongKong, China*

WP 629 **Automatic Top-Down Spectral Annotation of Modified Oligonucleotides**; Maria Basanta-sanchez[1]; Iggy Kass[2]; Catalin Doneanu[2]; *[1]Waters Corporation, Pleasanton, CA; [2]Waters Corporation, Milford, MA*

WP 630 **Discovery and Identification of an Unknown DNA Adduct in HeLa Cells Exposed to Colibactin-Producing E.coli using Untargeted DDA-CNL/MS3 Adductomic Analysis**; Peter W Villalta[1]; Matthew R Wilson[2]; Yindi Jiang[2]; Alessia Stornetta[1]; Paul D Boudreau[2]; Andrea Carra[1]; Caitlin A Brennan[3]; Eunyoung Chun[3]; Lizzie Ngo[4]; Leona D Samson[4]; Bevin P Engelward[4]; Wendy S Garrett[3,5,6]; Emily P Balskus[2]; Silvia Balbo[1,7]; *[1]University of Minnesota Masonic Cancer Center, Minneapolis, Minnesota; [2]Department of Chemistry and Chemical Biology, Harvard University, Cambridge, Massachusetts; [3]Department of Immunology and Infectious Diseases and Department of Genetics and Complex Diseases, Harvard T. H. Chan School of Public Health, Boston, Massachusetts; [4]Department of Biological Engineering, MIT, Cambridge, Massachusetts; [5]Broad Institute of MIT and Harvard, Cambridge, Massachusetts; [6]Department of Medical Oncology, Dana-Farber Cancer Institute, Boston, Massachusetts; [7]Division of Environmental Health Sciences, University of Minnesota, Minneapolis, Minnesota*

WP 631 **Method Development for Metabolite and Impurity Profiling of Oligonucleotide Therapeutics**; Kaoru Karasawa[1]; Lyle Burton[2]; Eva Duchoslav[2]; *[1]SCIEX, Shinagawa-ku, Japan; [2]SCIEX, Concord, ON*

WP 632 **Comparison between ISD by MALDI Tof and CID by ESI ion trap FTICR ofNF-κB Decoy Oligodeoxynucleotide and its metabolites**; Zenzaburo Tozuka[1]; Akihiro Kunisawa[2]; Junko Ilda[2]; Ryuichi Morishita[3]; Shohei Shioyama[4]; *[1]Grad. Sch. Pharm. Sci./ Osaka University, Suita, Osaka, Japan, Suita, Japan; [2]Anal. Innov. Res. Lab. Grad. Sch. Eng./ Osaka University, Suita, Japan; [3]Grad. Sch. Med. Sci./ Osaka University, Suita, Japan; [4]JCL Bioassay Corporation, Nishiwaki, Japan*

WP 633 **Study of the Reduction of Azidothymidine (AZT) Using Electrochemistry Coupled to a Mass Spectrometer**;

Raquel Teijeiro[1]; Francesca Cogliandro[1]; Elvira Gomez[1]; Jef Rozenski[1]; [1]*Rega Institute, Leuven, Belgium*

WP 634 **Identification and Characterization of Urinary Nucleosides using Compound Discoverer 3.0 and Fragment Identification Search (FISh)**; Robert Ross[1]; Ruoxia Zhao[1]; Ningxi Yu[1]; Andrew Wood[1]; Manasses Jora[1]; Ralf Tautenhahn[2]; Patrick A Limbach[1]; [1]*University of Cincinnati, Cincinnati, OH;* [2]*Thermo Fisher Scientific, San Jose, CA*

WP 635 **A Method for the Automated Determination of Early Eluting Oligonucleotide Drug Impurities Using IP-RPLC HRMS**; Stilianos G. Roussis[1]; Claus Rentel[1]; [1]*Ionis Pharmaceuticals, Inc., Carlsbad, CA*

WP 636 **Comparison of an Automated versus Manual SPE Sample Preparation Method for Improved Throughput during siRNA LC-MS Analysis**; Babak Basiri[1]; Thuy Tran[1]; Mark Boggeri[2]; Mei Han[1]; Fang Xie[1]; Brooke Rock[1]; [1]*Amgen Inc., South San Francisco, CA;* [2]*Tecan SP, Inc., Baldwin Park, CA*

WP 637 **Probing the Role of Specific Amino Acid Residues that Contribute to the Novel Ribonuclease Activity of Cusativin by LC-MS**; Priti Thakur[1]; Patrick A. Limbach[2]; Balasubrahmanyam Addepalli[2]; [1]*University of Cincinnati, Cincinnati , Ohio;* [2]*University of Cincinnati, Cincinnati*

WP 638 **A Highly Selective and Sensitive Analytical Method Using LC-MS/MS for Phosporothioate Oligonucleotides**; Yasuko Tsukazaki[1]; Naoto Senda[1]; Mariko Harada-Shiba[2]; Fumito Wada[2]; Noriyuki Iwasaki[3]; Kaoru Karasawa[3]; [1]*Shin Nippon Biomedical Laboratories, Ltd., Tsukuba, Japan;* [2]*National Cerebral and Cardiovascular Center Research Institute, Suita, Japan;* [3]*SCIEX, Shinagawa-ku, Japan*

WP 639 **Charge Deconvolution and Automatic Sequence Matching for Oligonucleotides**; Wilfred Tang[1]; Marshall Bern[1]; Rose D Lawler[1]; James Moore[1]; David Garby[2]; Nicholas Skizim[2]; [1]*Protein Metrics Inc., Cupertino, CA;* [2]*GreenLight Biosciences, Inc., Medford, MA*

WP 640 **Detection of the Altered tRNA Modification Profiles in Primary and Metastatic Melanoma by LC-MS**; Congliang Sun[1]; Zalfa Abdel-Malek[1]; Patrick A Limbach[1]; Balasubrahmanyam Addepalli[1]; [1]*University of Cincinnati, Cincinnati, OH*

WP 641 **Strategies for Bioanalysis of an Oligonucleotide and Chain-Shorted Metabolites from Human Plasma Employing LC-UV/MS/MS Detection**; Ying Peng[1]; Noah Post[2]; Moo-young Kim[1]; Shabana Khatri[2]; Shannon Hall[2]; Fumin Li[1]; [1]*PPD, Middleton, WI;* [2]*Ionis Pharmaceuticals, Inc., Carlsbad, CA*

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WP 642 **Glycoproteomic Analysis using 213 nm Ultraviolet Photodissociation Mass Spectrometry**; Edwin Escobar[1]; Jennifer S Brodbelt[1]; [1]*University of Texas at Austin, Austin, TX*

WP 643 **Simultaneous Glyco- and Phosphopeptide Enrichment by Phytic Acid-Modified Titanium(IV) Immobilized Metal Affinity Chromatography (PA-Ti-IMAC)**; Dylan Nicholas Tabang[1]; Yusi Cui[1]; Jillian Johnson[2]; Lingjun Li[1,2]; [1]*Department of Chemistry, University of Wisconsin, Madison, WI;* [2]*School of Pharmacy, University of Wisconsin, Madison, WI*

WP 644 **Identification of Glutamic Acid Isomers Produced During Deamidation Through RDD Diagnostic Fragments**; Jacob W Silzel[1]; Yana Lyon[1]; Dylan Riggs[1]; Ryan R. Julian[1]; [1]*UC Riverside, Riverside, CA*

WP 645 **Evaluation of an Automated, Acidic pH Protein Digestion for Reduced Levels of Artificial Deamidation in Biotherapeutic Peptide Mapping Studies**; Tom Buchanan[1]; Ken Cook[1]; Sara Carillo[2]; Silvia Millan Martin[2]; Dan Bach Kristensen[3]; Kevin Meyer[4]; Marc Geunder[5]; Rowan Moore[1]; [1]*Thermo Fisher Scientific, Runcorn, United Kingdom;* [2]*National Institute for Bioprocessing Research and Training, Dublin, Ireland;* [3]*Symphogen, Ballerup, Denmark;* [4]*Perfinity, West Lafayette, Indiana;* [5]*Thermo Fisher Scientific, Reinach, Switzerland*

WP 646 **Proteomic Analysis of Arginine-Rich RNA Binding Proteins by Electron Transfer Dissociation Mass Spectrometry**; Sean R Kundinger[1]; Isaac Bishof[1]; Duc M. Duong[1]; Nicholas T. Seyfried[1]; [1]*Emory University, Atlanta, GA*

WP 647 **Quantitative Proteomic Analysis of Histone-PTMs in Breast Cancer Stem Cells by Multiple Reaction Monitoring**; Seung Ju Moon[1]; Byoung-Kyu Cho[1]; Nu-Ri Im[1]; Eugene C. Yi[1]; [1]*Department of Molecular Medicine and Biopharmaceutical Sciences, Graduate School of Convergence Science and Technology, Seoul National University, Seoul, South Korea*

WP 648 **Novel Rabbit Monoclonal Antibodies for Profiling of Ser/Thr O-GlcNAc modified proteins**; Matthew D. Fry[1]; Rami Najjar[1]; Yiying Zhu[1]; Devin K Schweppe[2]; Steven Gygi[2]; Matthew P Stokes[1]; [1]*cell Signaling Technology, Danvers, MA;* [2]*Harvard Medical School, boston, MA*

WP 649 **Combining Proteomics Strategies to Study Polyglutamylated Peptides for Tubulin Analysis**; Thibault Chaze[1]; Mathieu Dupré[1]; Elise Warter[2]; Serge Bonnefoy[2]; Jujimon A.s[3]; Carsten Janke[3]; Philippe Bastin[2]; Mariette Matondo[1]; Julia Chamot-Rooke[1]; [1]*Mass Spectrometry for Biology Unit, Institut Pasteur, CNRS USR2000, Paris, France;* [2]*Trypanosome Cell Biology Unit, Institut Pasteur, INSERM U1201, Paris, France;* [3]*Regulation of Microtubule Dynamics and Functions Unit, Institut Curie, CNRS UMR3348, Orsay, France*

WP 650 **Delineation of Glycopeptides and D-Amino Acid Containing Peptides (DAACPs) with Variant PTM Structure or Localization by High-Resolution FAIMS and ETD**; Matthew A Baird[1]; Alexandre A Shvartsburg[1]; [1]*Wichita State University, Wichita, KS*

WP 651 **Large-Scale Profiling of Mannose-6-phosphate Glycoproteome from Human Cells by Ti(IV)-IMAC**; Danqing Wang[1]; Junfeng Huang[2]; Yuan Liu[2]; Yusi Cui[1]; Jillian Johnson[2]; Lingjun Li[1,2]; [1]*Department of Chemistry, University of Wisconsin-Madison, Madison, WI 53706;* [2]*School of Pharmacy, University of Wisconsin-Madison, Madison, WI 53705*

WP 652 **Optimized EThcD Fragmentation Method for Confirmation of Isoaspartic Acid Peptides**; Raghothama Chaerkady[1]; Ben Niu[1]; Keith Rickert[1]; Sonja Hess[1]; [1]*MedImmune, Gaithersburg*

WP 653 **Expanding the Glycoforms Detected in Complex Glycopeptide Datasets**; Katalin F. Medzihradszky[1]; Peter R. Baker[2]; Adam Pap[1]; Zsuzsanna Darula[1]; Robert Chalkley[2]; [1]*Biological Research Centre of the Hungarian Academy of Sciences, Szeged, Hungary;* [2]*UCSF, San Francisco, CA*

WP 654 **Highly Efficient and Precise Glycoproteomic Analysis with Intelligent Technology**; Weiqian Cao[1]; Wenfeng Zeng[2]; Mingqi Liu[1]; Chao Liu[2]; Biyun Jiang[1]; Pan Fang[1]; Huali Shen[1]; Simin He[2]; Pengyuan Yang[1]; [1]*Fudan University, Shanghai, China;* [2]*Institute of Computing Technology, Chinese Academy of Sciences, Beijing, China*

WP 655 **A Novel, Fast Post Translational Modification Localization Algorithm for Targeted DIA Outperforming DDA on a Controlled Sample Set**; Oliver M Bernhardt[1]; Christian D. Kelstrup[2]; Tejas Gandhi[1]; Lynn Verbeke[1]; Alexander Hogrebe[3]; Dorte B. Bekker-Jensen[2]; Jesper V. Olsen[3]; Lukas Reiter[1]; [1]*Biognosys AG, Schlieren, Switzerland;* [2]*Novo Nordisk Foundation Center for Protein Research, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark;* [3]*Novo Nordisk Foundation Center for Protein Research, Faculty*

of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark

WP 656 **Finding the Sweet Spot in SAX-ERLIC Mobile Phase for Simultaneous Enrichment of Glyco and Phospho-peptides**; Yusi Cui[1]; Ka Yang[2]; Dylan Nicholas Tabang[2]; Junfeng Huang[2]; Weiping Tang[2]; Lingjun Li[2]; *[1]University of Wisconsin-Madison, Madison, WI; [2]University of Wisconsin, Madison, Madison, WI*

WP 657 **RDD-MS Reveals the Isomerization Rate of Amyloid Beta and a Novel Cause for Alzheimer's Disease**; Ryan R. Julian[1]; Dylan Riggs[1]; Tyler Lambeth[1]; *[1]University of California, Riverside, Riverside, CA*

WP 658 **Verification of Sulfotyrosine and 4-Hydroxyproline in Biotherapeutics**; Oksana Tyshchuk[1]; Christoph J. Gstöttner[2]; Dennis Funk[3]; Simone Simone Nicolardi[2]; Stefan Frost[3]; Felix Schumacher[3]; Manfred Wuhrer[2]; Michael Molhoj[3]; Vincent Larraillet[3]; *[1]Roche Diagnostics GmbH, Penzberg, Germany; [2]Leiden University Medical Center, Center for Proteomics and Metabolomics, Leiden, Netherlands; [3]Roche Pharmaceutical Research and Early Development (pRED), Roche Innovation Center Munich, Germany*

WP 659 **Intergrated Mass Spectrometry Method Development for Arginine methylation Analysis**; Chao Peng[1]; Ping wu[2]; *[1]National Center for Protein Science (Shanghai), Institute of Biochemistry and Cell biology, SIBS, CAS, Shanghai, China; [2]National facility for Protein Science, Shanghai, China*

WP 660 **Comparison of Enrichment Strategies for the In-Depth Proteomics Analysis of ADP-Ribosylation Sites**; Alexandra F. Stripp[1]; Sara C. Larsen[1]; Ivo A. Hendriks[1]; Michael L. Nielsen[1]; *[1]Novo Nordisk Foundation Center for Protein Research, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark*

WP 661 **Investigating Crosstalk between endogenous SUMOylation and ADP-Ribosylation in the Cellular Response to Oxidative Stress**; Ivo A. Hendriks[1]; Michael L. Nielsen[1]; *[1]Novo Nordisk Foundation Center for Protein Research, Faculty of Health and Medical Sciences, University of Copenhagen, Copenhagen, Denmark*

WP 662 **Identification and Quantitation of Phosphopeptide Positional Isomers using Trapped Ion Mobility Spectrometry and PASEF**; Chris Adams[1]; Michael Krawitzky[1]; Katherine Tran[2]; Baozhen Shan[2]; Zac Anderson[2]; Charles Farnsworth[3]; Matthew P Stokes[3]; Kimberly Lee[3]; Shourjo Ghose[4]; Matthew Willetts[4]; Gary Kruppa[4]; *[1]Bruker Daltonics, San Jose, CA; [2]Bioinformatics Solutions Inc., Waterloo, ON; [3]Cell Signaling Technology, Danvers, MA; [4]Bruker Daltonics Inc., Billerica, MA*

WP 663 **Characterization and Discrimination of Sulfopeptides and Phosphopeptides in Positive Mode Mass Spectrometry**; Maia Kelly[1]; Justin Lawrie[1]; Jiantao Guo[1]; Eric D. Dodds[1]; *[1]University of Nebraska - Lincoln, Lincoln, NE*

WP 664 **Supercharging of Palmitoylated Peptides for Improved Electron Capture/Transfer Dissociation Tandem Mass Spectrometry**; Nhat H.V. Le[1]; John E. Crellin[1]; Gabriela Grigorean[1]; Brent R. Martin[1]; Kristina Hakansson[1]; *[1]University of Michigan, Ann Arbor, MI*

WP 665 **Direct Identification and Site-Specific Profiling of S-Palmitoylation by Liquid Chromatography/Tandem Mass Spectrometry**; John E. Crellin[1]; Nicholas B. Borotto[1]; Krisitina Hakansson[1]; Brent R. Martin[1]; *[1]University of Michigan, Ann Arbor, MI*

WP 666 **Identification of γ-Carboxyglutamic Acid Modified Proteins in Triple Negative Breast Cancer Cells by Immunocapture and Data Dependent nanoLC-MS/MS**; James McCardle[1,2]; Sarah Beaudin[2]; Leila Kokabee[2]; JoEllen Welsh[1,2]; *[1]School of Public Health, Rensselaer, NY; [2]University at Albany-SUNY, Rensselaer, NY 12144*

WP 667 **Identification of Human Chorionic Gonadotropin Glycoforms in Two Populations Using Improved Bottom-Up Analysis**; Nicolas Eskenazi[1]; Chiara Giangrande[1]; Joëlle Vinh[1]; *[1]SMBP, ESPCI, PSL University, Paris, France*

WP 668 **Identifying the Range of Protein Post-Translational Modifications that have Temporal Rhythms in the CAM Plant Kalanchoe**; Cheng Chen[1]; Paul Abraham[1,2]; Robert Hettich[1,2]; *[1]University of Tennessee, Knoxville, TN; [2]Oak Ridge National Laboratory, Oak Ridge, TN*

WP 669 **Comprehensive Profiling of ADP-Ribosylation Sites Using Complementary Proteolytic Digestion and Precursor Fragmentation Strategies**; Sara C Larsen[1]; Ivo A. Hendriks[1]; Michael L. Nielsen[1]; *[1]University of Copenhagen NNF CPR, Copenhagen N, Denmark*

WP 670 **Unstructured Regions are Hotspots of Arginine Dimethylation in Neurodegeneration-Linked Proteins**; Jeremy D. O'Connell[1]; Janos Demeter[1]; Marcus Kelly[1]; Nancie A. Mooney[1]; Ran Cheng[1]; Peter K. Jackson[1]; *[1]Stanford University, Palo Alto, CA*

WP 671 **Screening Spectra from Dimethylated Peptides Improve the Identification Rate of SUMOylation Sites by Orbitrap Mass Spectrometer**; Fu-An Li[1]; Yu-Hsiang Cheng[1]; *[1]Institute of Biomedical Sciences, Academia Sinica, Taipei, Taiwan*

WP 672 **Database Search Strategies for Sulfopeptide Identification**; Hye Kyong Kweon[1]; Andy T. Kong[2]; Katherine E. Hersberger[1]; Shijiao Huang[1]; Yanzhuang Wang[1]; Alexey I. Nesvizhskii[2]; Philip C. Andrews[1]; Kristina Hakansson[1]; *[1]University of Michigan, Ann Arbor, MI; [2]University of Michigan Medical School, Ann Arbor, MI*

WP 673 **Assessment of Chromatographic Separation and Fragmentation Behavior of Isobaric Phosphopeptides Using Data Independent Acquisition Mass Spectrometric Approaches**; Christian A Doerig[1]; Ludovic Gillet[1]; Ulrike Kusebauch[2]; Dave Lee[3]; Robert L Moritz[2]; Anthony D Whetton[3,4]; Paola Picotti[1]; Ruedi Aebersold[1,5]; *[1]Department of Biology, Institute of Molecular Systems Biology, ETH Zurich, Zurich, Switzerland; [2]Systems Biology, Seattle, WA; [3]Stoller Biomarker Discovery Centre, University of Manchester, Manchester, United Kingdom; [4]The School of Medical Sciences and Manchester Academic Health Sciences Centre, University of Manchester, Manchester, United Kingdom; [5]Faculty of Science, University of Zurich, Zurich, Switzerland*

WP 674 **Pinpointing Isomerization Sites in Human Lens Crystallin using IMS-MS**; Hoi Ting Wu[1]; Ryan R. Julian[1]; *[1]University of California, Riverside, Riverside, CA*

WP 675 **Identification of Cross-Linked Peptides and Oxidation Products in Lysozyme Subjected to Photo-Oxidation and Peroxyl Radical Oxidation**; Michele Mariotti[1]; Eduardo Fuentes-Lemus[2]; Camilo López Alarcón[2]; Per Hägglund[3]; Michael Jonathan Davies[3]; *[1]University of Copenhagen, Copenhagen, Denmark; [2]University of Chile, Santiago, Chile; [3]University of Copenhagen, Copenhagen, Denmark*

PEPTIDES: TARGETED AND QUANTITATIVE ANALYSIS
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WP 676 **Blood Brain Barrier (BBB) Penetration of Pituitary Adenylate Cyclase-Activating Polypeptide (PACAP) Glycosylated Peptides by 'Shotgun Microdialysis' Coupled with LC-MS3**; Chenxi Liu[1]; Mitchell J Bartlett[2]; Christopher Robert Apostol[1]; Lajos Szabo[1]; Robin Polt[1]; Torsten Falk[2]; Michael L Heien[1]; *[1]Department of Chemistry and Biochemistry, The University of Arizona, Tucson, Arizona; [2]Department of Neurology, The University of Arizona, Tucson, Arizona*

WP 677 **Targeted Quantification of Detergent-Insoluble RNA-Binding Proteins in Alzheimer's Diseases**; Qi Guo[1]; Eric B Dammer[1]; maotian zhou[1]; Marla Gearing[1]; James J.

Lah[1]; Allan I. Levey[1]; Nicholas Seyfried[1]; [1]*Emory University, Atlanta, GA*

WP 678 **Quantification of a Novel Peptide, CPT31, in Rat and Monkey Plasma by LC-MS**; China Y. Lim[1]; Sarah Meghan Kriger[1]; Brandon Wilcock[1]; Vamshi Manda[1]; Brett Welch[2]; Erik Kish-Trier[3]; Scott Reuschel[1]; Troy Voelker[1]; [1]*Covance, Salt Lake City, UT;* [2]*Navigen, Inc., Salt Lake City, UT;* [3]*ARUP Laboratories, Salt Lake City, UT*

WP 679 **A Comparison Between MRM and PRM for the Quantitation of LEAP2 in Serum**; Chelsea C. Boo[1]; Ranjitha Gaddipati[1]; Joseph S. Grimsby[1]; Sonja Hess[1]; [1]*MedImmune, Gaithersburg, MD*

WP 680 **Developing a Targeted Method for Monitoring Cytosolic Iron-Sulfur Cluster Assembly Pathway**; Xiaorui Fan[1]; William D. Barshop[1]; Ajay A. Vashisht[1,2]; Stephanie Leal[3]; James A. Wohlschlegel[1]; [1]*UCLA, Los Angeles, CA;* [2]*The Genomics Institute of the Novartis Research Foundation, San Diego, CA;* [3]*California State University-Long Beach, Long Beach, CA*

WP 681 **Sub-Picogram Level Quantitation of Desmopressin in Small Volumes of Human Plasma Using a Trap-Elute Micro LC-MS System**; Rahul Baghla[1]; Khatereh Motamedchaboki[1]; Remco van Soest[1]; Lei Xiong[1]; [1]*Sciex, Redwood City, CA*

WP 682 **A Potential Reference Measurement Procedure for Quantification of α-Synuclein in Biological Fluids**; Julia Mateyka[1]; Adam Cryar[1]; Giles Drinkwater[1]; Milena Quaglia[1]; Guglielmo Verona[2]; Vittorio Bellotti[2]; Sylvain Lehmann[3]; [1]*LGC Group, Teddington, United Kingdom;* [2]*UCL, London, United Kingdom;* [3]*CHU Montpellier, Montpellier, France*

WP 683 **A Software Platform for Peptide Synthesis Quality Control by both LC-free MALDI-TOF and LC-ESI-QTOF Molecular Weight Determination**; Anjali Alving[1]; Eckhard Belau[2]; Waltraud Evers[2]; Anja Resemann[2]; Wulff Niedner[2]; Detlev Suckau[2]; [1]*Bruker Daltonics Inc., Billerica, MA;* [2]*Bruker Daltonics, Bremen, Germany*

WP 684 **Factors that Influence the Recovery of Hydrophobic Peptides during LC-MS Sample Handling**; Moon Chul Jung[1]; Kim Haynes[1]; Markus Wanninger[1]; [1]*Waters Corporation, Milford, MA*

WP 685 **Absolute Quantification of Targeted Host Cell Proteins (HCPs) in Biotherapeutics by Liquid Chromatography-Multiple Reaction Monitoring (LC-MRM) Method**; Baibhav Rawal[1]; Xnliu Gao[2]; Yan-Hui Liu[2]; [1]*Merck & Co., Kenilworth, NJ;* [2]*Merck & Co. Inc., Kenilworth, New Jersey*

WP 686 **Sequential Windowed Acquisition of Reporter Masses for Quantitation-First Proteomics**; William D. Barshop[1]; Hee Jong Kim[1]; Shima Rayatpisheh[1]; James A. Wohlschlegel[1]; [1]*University of California Los Angeles, Los Angeles, CA*

WP 687 **Gonadotropin-Releasing Hormones (GnRH) Quantitation in Brain and Plasma by LC-HRMS/MS**; Claudio Medana[1]; Federica Dal Bello[1]; Michael Zorzi[1]; Elisa Pastorello[1]; Paolo Giacobini[2]; [1]*University of Turin, Torino, Italy;* [2]*Inserm, Lille, France*

WP 688 **Developing Fit-for-Purpose LC-MS Based Quantitative Assays to Support Drug Discovery Activities for Cyclic Peptides**; Rena N Zhang[1]; Michelle R Robinson[2]; Komal Kedia[2]; Daniel Spellman[2]; [1]*Merck & Co., Inc, West Point, PA;* [2]*Merck & Co., Inc., West Point, PA*

WP 689 **Detecting Low Abundance Proteins in the Complex Background of the Cochlea by Mass Spectrometry**; Miguel Ramirez; *Northwestern University, Chicago, IL*

WP 690 **Quantification and Evaluation of Sample Preparation Techniques in the Determination of Dynorphin Opioid Peptides by LC-MS/MS (MRM)**; Karthik Chandu[1]; Tony L Sahley[2]; Michael D Hammonds[2]; Masaru Miyagi[3]; David J Anderson[4]; [1]*Cleveland State University, Cleveland, OH;* [2]*School of Health Sciences; Cleveland State University, Cleveland, OH;* [3]*Department of Pharmacology; Case Western Reserve University, Cleveland, OH;* [4]*Department of Chemistry; Cleveland State University, Cleveland, OH*

WP 691 **The Role of the Cytoplasmic Capping Enzyme on the Proteome Diversity**; Bernice A. Agana[1]; Sophie R. Harvey[1]; Daniel R. Schoenberg[1]; Vicki H. Wysocki[1]; [1]*The Ohio State University, Columbus, OH*

WP 692 **Assay of Human Insulin by Liquid Chromatography High Resolution Mass Spectrometry**; Kui Zeng[1]; Jingyue Yang[1]; Connie Ruzicka[1]; [1]*FDA, Saint Louis, MO*

WP 693 **Retention Time Correction Method Utilizing Unspecified Peaks in MS Scans**; Philip M Remes[1]; Ping Yip[1]; Romain Huguet[1]; [1]*Thermo Fisher Scientific, San Jose, CA*

WP 694 **Targeted Top-down Mass Spectrometry for Characterization and Quantitation of Crustacean Hyperglycemic Hormones (CHHs) and CHH Precursor-Related Peptides**; Yang Liu[1]; Gongyu Li[1]; Lingjun Li[1]; [1]*University of Wisconsin-Madison, Madison, WI*

WP 695 **Investigations of *Caenorhabditis elegans* egl-3 Mutants Reveal an Important Role in Neuropeptide Processing and a Significant Impact on Nocifensive Responses**; Bruno Nkambeu[1]; Jennifer Ben Salem[1,2]; Dina N Arvanitis[2]; Francis Beaudry[1]; [1]*Universite de Montreal, St-Hyacinthe, QC;* [2]*Institut des Maladies Métaboliques et Cardiovasculaires, INSERM UMR1048, Toulouse, France*

WP 696 **Development of a high throughput hybrid MS assay for human insulin in clinical samples, using surrogate matrices**; Michael A. Blackburn[1]; Stuart McDougall[1]; Stephen Gray[1]; [1]*Arcinova, Northumberland, United Kingdom*

WP 697 **Verification of the Bladder Cancer Biomarker Candidates in Clinical Urine Specimens by a SISCAPA-MRM Assay**; Yi-Ting Chen[1]; Meng-Kai Chou[1]; Yung-Chin Hsiao[1]; Ying-Hsu Chang[2]; Chien-Lun Chen[2]; Jau-Song Yu[1]; Yu-Sun Chang[1]; [1]*Chang Gung University, Taoyuan, Taiwan;* [2]*LinKou Chang Gung Memorial Hospital, Taoyuan, Taiwan*

WP 698 **Podocalyxin and Podocin Multiplex Urine Analysis using Tandem Mass Spectrometry for the Evaluation of Podocyturia in Patients**; Tristan Martineau[1]; Michel Boutin[1]; Anne-Marie Côté[1]; Daniel Bichet[2]; Bruno Maranda[1]; Christiane Auray-Blais[1]; [1]*Université de Sherbrooke, Sherbrooke, QC;* [2]*Hôpital du Sacré-Cœur, Université de Montréal, Montréal, QC*

WP 699 **A Comparative Study on Peptide Quantitation between Traditional LC-MS/MS and microLC-MS/MS for Discovery DMPK**; Yuanqiang Su[1]; Meijuan He[1]; Xinxin Wen[1]; Xiaotong Li[1]; Cheng Chen[1]; Weimin Hu[1]; Weiqun Cao[1]; Lili Xing[1]; Xin Zhang[1]; Yi Tao[1]; [1]*WuXi AppTec, Shanghai, China*

WP 700 **Towards Turnkey Targeted Proteomics Solutions using Internal Standard Triggered Acquisitions on Modified Orbitrap Mass Spectrometers**; Sebastien Gallien[1,2]; Aaron S. Gajadhar[3]; Bhavin Patel[4]; Markus Kellmann[5]; Tabiwang N. Arrey[5]; Alexander Harder[5]; Romain Huguet[3]; Graeme McAlister[3]; Derek Bailey[3]; Shannon Eliuk[3]; Emily I. Chen[1]; Yue Xuan[5]; Andreas Huhmer[3]; [1]*Thermo Fisher Scientific, Precision Medicine Science Center, Cambridge, MA;* [2]*Thermo Fisher Scientific, Paris, France;* [3]*Thermo Fisher Scientific, San Jose, CA;* [4]*Thermo Fisher Scientific, Rockford, IL;* [5]*Thermo Fisher Scientific, Bremen, Germany*

WP 701 **Comparison of Targeted Proteomics Approaches on a TIMS-Q-TOF**; Antoine Lesur[1]; Pierre-Olivier Schmit[2]; Joseph Longworth[1]; Gunnar Dittmar[1]; [1]*LIH, Luxembourg Institute of Health, Strassen, Luxembourg;* [2]*Bruker Daltonique S.A., Wissembourg, France*

WP 702 **Targeted Membrane Protein Quantification for Therapeutic Target Identification**; Lei Guo; *Sanofi, Cambridge, MA*

WP 703 **Development of a Very Sensitive LC-MS Assay to Quantitate Ultra Low Levels of GLP-1 Targeted Peptide Mimetics**; Jennifer Luong[1]; Jeremy Brassard[1]; Alyssa Kabat[1]; Eric Schnieder[2]; Allysen Meymaris[1]; Steven Wiltshire[1]; Jakal Amin[1]; *[1]Charles River Laboratories, Worcester, MA; [2]ProLynx LLC, San Francisco, CA*

PROTEINS: COMPLEXES/NON-COVALENT INTERACTIONS I
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WP 704 ***In-situ* Chemical X-linking MS for Antibody-tractable Antigen identification**; Kang Hyun Kim[1]; Jung Hyeon Lee[2]; Seung Ju Moon[1]; Kristine M. Kim[2]; Eugene C. Yi[1]; *[1]Department of Molecular Medicine and Biopharmaceutical Sciences, Graduate School of Convergence Science and Technology, Seoul National University, Seoul, South Korea; [2]Division of Biomedical Convergence, College of Biomedical Science, Kangwon National University, Chuncheon, South Korea*

WP 705 **Multiplexed TMT-Based Interactomics Reveals Coordination of Proteostasis Network Remodeling and Mechanisms of Protein Quality Control**; Madison T Wright[1]; Lars Plate[1]; *[1]Vanderbilt University, Nashville, TN*

WP 706 **Revealing the Molecular Makeup of Rationally Designed Heteroligomeric Assemblies of Stable Protein 1**; Nicholas Demarais; *University of Auckland, Auckland, New Zealand*

WP 707 **Thyroglobulin as a Model for Analysis of Protein Quality Control Dynamics**; Madison T. Wright[1]; Lars Plate[1]; *[1]Vanderbilt University, Nashville, TN*

WP 708 **TRIM28 as a Candidate Mutant p53 Interacting Partner in Cancer Cells**; Mariel R Mendoza[1]; Katherine Alexander[1]; Enrique Lin Shiao[1]; Charly Ryan Good[1]; Benjamin A. Garcia[1]; Shelley L. Berger[1]; *[1]University of Pennsylvania, Philadelphia*

WP 709 **Analysis of the Lysosomal Membrane Interactome via Cross-Linking Mass-Spectrometry**; Jasjot Singh[1]; Srigayatri Ponnaiyan[1]; Fatema Akter[1]; Dominic Winter[1]; *[1]University of Bonn - Institute of Biochemistry and Molecular Biology, Bonn, Germany*

WP 710 **FBXO11 Network Identifies Novel Disease-Relevant Interaction with the Ubiquitin-Specific Protease USP28**; Jonathan St-Germain[1]; Etienne Coyaud[1]; Estelle Laurent[1]; Faith Yeung[1]; Brian Raught[1]; *[1]Princess Margaret Cancer Centre, Toronto, ON*

WP 711 **Chaperone Activation and Client Binding of a 2-Cysteine Peroxiredoxin as Determined by Crosslinking Combined with MS and Cryogenic Electron Microscopy**; Karl A. T. Makepeace[1,2]; Filipa Teixeira[3,4,5,6]; Eric Tse[7]; Helena Castro[4,6]; Ben A. Meinen[4,6]; Leslie B. Poole[9]; James C. Bardwell[3,8]; Ana M. Tomás[4,5,6]; Evgeniy V. Petrotchenko[10]; Daniel R. Southworth[7]; Ursula Jakob[3]; Christoph H. Borchers[1,2,10,11]; *[1]University of Victoria-Genome BC Proteomics Centre, Victoria, BC; [2]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; [3]Department of Molecular, Cellular, and Developmental Biology, Ann Arbor, Michigan; [4]i3S - Instituto de Investigação e Inovação em Saúde, Universidade do Porto, Porto, Portugal; [5]IBMC - Instituto de Biologia Molecular e Celular, Universidade do Porto, Porto, Portugal; [6]ICBAS – Instituto de Ciências Biomédicas Abel Salazar, Universidade do Porto, Porto, Portugal; [7]Department of Biochemistry and Biophysics, Institute for Neurodegenerative Diseases, University of California, San Francisco, CA; [8]Howard Hughes Medical Institute, University of Michigan, Ann Arbor, Michigan; [9]Wake Forest Baptist Medical Center, Winston-Salem, NC; [10]Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; [11]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC*

WP 712 **Mass Spectrometry-Based Protein Footprinting Probes the Conformational Changes during Aβ42 Aggregation upon Binding to Novel Small Molecule Inhibitors**; Saketh Chemuru[1]; George Mathai[2]; Jong Hee Song[1]; Michael L Gross[1]; *[1]Washington University, St.louis, MO; [2]Sacred Heart College, Cochin, India*

WP 713 **On the Possibility of an Idiosyncratic Role of Heparin as Anticoagulant: *in vitro* Deactivation of Factor Xa via Heparin-Assisted Autolysis**; Chendi Niu[1]; Cedric E. Bobst[1]; Sergey Savinov[1]; Igor A. Kaltashov[1]; *[1]University of Massachusetts Amherst, Amherst, MA*

WP 714 **Native Top Down Analysis of 184-218 kDa Protein Complexes Reveals the First Pentameric Viral Fibrils**; Matthew V. Holt[1]; Tao Wang[1]; Nicolas Leon Young[1]; *[1]Baylor College of Medicine, Houston, TX*

WP 715 **Rapid and Automatable Desalting of Protein Complexes by Size Exclusion Chromatography for On-line Detection by Native Mass Spectrometry**; Zachary VanAernum[1,2]; Florian Busch[1,2,3]; Benjamin J. Jones[1,2]; Mengxuan Jia[1,2]; Vicki Wysocki[1,2,3]; *[1]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, Ohio; [2]Resource for Native Mass Spectrometry Guided Structural Biology, Columbus, OH; [3]Campus Chemical Instrument Center, The Ohio State University, Columbus, Ohio*

WP 716 **Investigating the Glycan Ligands of Siglecs through MS-Based Shotgun Glycomics**; Heajin Park[1]; Elena N Kitova[1]; Jaesoo Jung[1]; Emily Rodrigues[1]; Matthew S. Macauley[1]; John Klassen[1]; *[1]University of Alberta, Edmonton, AB*

WP 717 **A Cross-Linking-Aided IP/MS Workflow Reveals Extensive Intracellular Trafficking in Time-Resolved, Signal-Dependent EGFR Proteome**; Yue Chen[1]; Mei Leng[1]; Yankun Gao[2]; Jongmin Choi[1]; Dongdong Zhan[2]; Jun Qin[1,2]; Sung Yun Jung[1]; Yi Wang[1,2]; *[1]Department of Biochemistry and Molecular Biology, Baylor College of Medicine, Houston, TX; [2]National Center for Protein Sciences (Beijing), State Key Laboratory of Proteomics, Institute of Lifeomics, Beijing, China*

WP 718 **Characterization of Essential Reprogramming Factors' Interaction Partner Dynamics during Cellular Reprogramming towards Pluripotency through Multiple Optimized Proteomics Approaches**; Weixian Deng[1]; William Barshop[1]; *[1]UCLA, Los Angeles, CA*

WP 719 **Tandem Ion Mobility Coupled with Mass Spectrometry for Gas Phase Protein Unfolding Studies**; LeRoy B Martin[1]; Martin Palmer[2]; Dale A Cooper-Shepherd[2]; James I Langridge[2]; *[1]Waters Corporation, Beverly, MA; [2]Waters Corporation, Wilmslow, United Kingdom*

WP 720 **Characterization of Protein Biotinylation Sites by Peptide-Based Immunoaffinity Enrichment**; Yiying Zhu[1]; Matthew D. Fry[1]; Alissa J. Nelson[1]; Jianmin Ren[1]; Vicky Yang[1]; Michael C. Palazzola[1]; Charles L. Farnsworth[1]; Matthew P. Stokes[1]; Kimberly A. Lee[1]; *[1]Cell Signaling Technology, Danvers, MA*

PROTEOMICS: QUANTITATIVE III
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WP 721 **Integrated Quantitative Proteomics in Cardiac Regeneration for Cardiac Systems Biology**; Trisha Tucholski[1]; Ling Gao[2]; Kyle Brown[1]; Yanlong Zhu[1]; Jake Melby[1]; Jianyi Zhang[2]; Ying Ge[1]; *[1]University of Wisconsin, Madison, WI; [2]University of Alabama at Birmingham, Birmingham, AL*

WP 722 **A "GeLC-MS"-Based Method for Label-Free Quantitative Proteomics of Bronchoalveolar Lavage Fluid following Diisocyanate Exposure**; Brandon F. Law[1]; Chen-Chung Lin[1]; Justin M. Hettick[1]; *[1]NIOSH, Morgantown, WV*

WP 723 **Exploring Egg Characteristics of Striped Bass**; Taufika Islam Williams[1]; Cara Kowalchyk[1]; Jesse Fischer[1]; Benjamin J. Reading[1]; *[1]North Carolina State University, Raleigh, NC*

WP 724 **Development of Label Free Quantitative Method for Proteomics and its Validation through Interlab Study;** Ki Na Yun[1,2]; Geul Bang[1,3]; Gun Wook Park[1]; Heeyoun Hwang[1]; Hongkyeong Jung[1]; Hye-Jung Kim[4]; Eugene Lee[5]; Yong-In Kim[5]; Jeong Hee Moon[6]; Sungho Yun[7]; Jong Shin Yoo[1]; Jin Young Kim[1]; *[1]Biomedical Omics Group, Korea Basic Science Institute, Cheongju, South Korea; [2]Department of Chemistry, Sogang University, Mapo-gu, South Korea; [3]College of Pharmacy, Korea University, Jochiwon, South Korea; [4]New Drug Development Center, KBIO Osong Medical Innovation Foundation, Cheongju, South Korea; [5]Korea Research Institute of Standards and Science, Yuseong-gu, South Korea; [6]Disease Target Structure Research Center, KRIBB, Yuseong-gu, South Korea; [7]Drug and disease target research team, Korea Basic Science Institute, Cheongju, South Korea*

WP 725 **Isotope Dilution Mass Spectrometry for Quantification of Influenza Proteins in Various Influenza Virus Preparations and Vaccines;** Wanda I Santana[1]; Lidoshka Marc[1]; Hans C Cooper[1]; John R Barr[1]; Tracie L Williams[1]; *[1]Centers for Disease Control and Prevention, Atlanta, GA*

WP 726 **A Proteomic-Based Pathway Analysis Identifies Bmi1 as a Potential Modulator for Tumor Growth and Invasion in Triple Negative Breast Cancer;** JungHun Lee[1]; Bobae Shim[2]; Hyeyoon Kim[1,2]; Han Suk Ryu[2]; Dohyun Han[1]; *[1]Proteomics core facility, Biomedical Research Institute, Seoul National University Hospital, Seoul, South Korea; [2]Department of Pathology, Seoul National University Hospital, Seoul National University College of Medicine, Seoul, South Korea*

WP 727 **Proteomics Investigation of Induced Obstructive Sleep Apnea (OSA) in Rat Atria using Mass Spectrometry;** Devika Channaveerappa[1]; Jacob C. Lux[1]; Madhuri Jayathirtha[1]; Cristiana Dumbraveanu[1]; Brian K. Panama[2]; Costel C. Darie[1]; *[1]Clarkson University, Potsdam, NY; [2]Masonic Medical Research Laboratory, Utica, NY*

WP 728 **Quantitative Proteomics of Acetomicrobium hydrogeniformans OS1: Converting Glucose to H2;** Janine Y. Fu[1]; Lauren Cook[1]; Farzaneh Sedighian[1]; Matthew Maune[2]; Ralph S. Tanner[2]; Michael J. McInerney[2]; Joseph A. Loo[1]; Robert P. Gunsalus[1]; Rachel R. Ogorzalek Loo[1]; *[1]University of California Los Angeles, Los Angeles, CA; [2]University of Oklahoma, Norman, OK*

WP 729 **A Comprehensive Characterization of Proteome in Sz. Pombe DJ-1 Homologs: a Preliminary Study;** aline De Lima Leite[1,2]; Kaleb Jones[1]; Eli Riekeberg[1]; Mark Wilson[1,2]; Robert Powers[1,2,3]; *[1]University of Nebraska Lincoln, Lincoln, NE; [2]Nebraska Center for Integrated Biomolecular Communication, University of Nebraska-Lincoln, Lincoln, Nebraska; [3]Redox Biology Center, University of Nebraska-Lincoln, Lincoln, Nebraska*

WP 730 **Meltome Atlas – Thermal Proteome Stability across the Tree of Life;** Anna Jarzab[1]; Nils Kurzawa[2]; Thomas Hopf[3]; Matthias Moerch[4]; Jana Zecha[1]; Niels Leijten[5]; Eva Musiol[6]; Melanie Maschberger[3]; Gabrielle Stoehr[3]; Charlotte Daly[1]; Tobias Schmidt[1]; Julia Mergner[1]; Britta Spanier[7]; Angel Angelov[4]; Thilo Werner[8]; Marcus Bantscheff[9]; Mathias Wilhelm[1]; Martin Klingenspor[6]; Simone Lemeer[9]; Wolfgang Liebl[4]; Hannes Hahne[3]; Mikhail Savitski[10]; Bernhard Kuster[1]; *[1]Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany; [2]Genome Biology Unit, EMBL Heidelberg, Heidelberg, Germany; [3]OmicScouts GmbH, Freising, Germany; [4]Department of Microbiology, Technical University of Munich, Freising, Germany; [5]Netherlands Proteomics Center, Utrecht, Netherlands; [6]Chair of Molecular Nutritional Medicine, Technical University of Munich, Freising, Germany; [7]Molecular Nutrition Unit, Technical University of Munich, Freising, Germany; [8]Cellzome, a GSK company, Heidelberg, Germany; [9]Netherlands Proteomics Center, Utrecht, Netherlands; [10]Genome Biology Unit, EMBL Heidelberg, Germany, Heidelberg, Germany*

WP 731 **Doxorubicin-Induced Changes in the HLA Peptidome Determined using Tandem Mass Tags;** Patrick Murphy[1]; Prathyusha Konda[1]; Joao A. Paulo[2]; Heiko Schuster[3]; Daniel J Kowalewski[3]; Youra Kim[1]; Derek R Clements[1]; Michael Giacomantonio[1]; Stefan Stevanović[3]; Steven P Gygi[2]; Shashi Gujar[1]; *[1]Dalhousie University, Halifax; [2]Harvard Medical School, Boston, MA; [3]Tuebingen University, Tuebingen, Germany*

WP 732 **Various Gonadotrohin Amounts Have Different Influence on the Secretom of human Granulosa and KGN Cells;** Tanja Panic-Jankovic[1]; Ulrike Resch[2]; Goran Mitulovic[1]; *[1]Medical University of Vienna, Vienna, Austria; [2]Medical University of Vienna, Vienna, Austria*

WP 733 **Quantitative Analysis of Chromatin Bound Metabolic Enzymes by High Resolution Mass Spectrometry;** Katja Parapatics[1]; Jung-Ming George Lin[2,3]; Sara Sdelci[2]; Andre C. Müller[2]; Stefan Kubicek[2,3]; *[1]CeMM-Research Center for Molecular Medicine of the Austrian Academy of Sciences, Vienna, Austria; [2]CeMM-Research Center for Molecular Medicine of the Austrian Academy of Sciences, Vienna, Austria; [3]Christian Doppler Laboratory for Chemical Epigenetics and Antiinfectives, CeMM Research Center for Molecular Medicine of the Austrian Academy of Sciences, Vienna, Austria*

WP 734 **Data Analysis for Accurate Label-Free Quantitation: Detection of and Correction for Co-Eluting Peptides;** Wenzhu Zhang[1]; Brian T. Chait[1]; *[1]The Rockefeller University, New York, NY*

WP 735 **Optimizing Injection Time Predictions to Improve Isobaric Reagent Reporter Ion Yield during Multiplexed Quantitative Proteomic Experiments;** Craig Braun[1]; Ryan Kunz[1]; Alison Erickson[1]; Steven P Gygi[2]; Brian Erickson[1]; *[1]IQ Proteomics LLC, Cambridge, MA; [2]Harvard Medical School, Boston, MA*

WP 736 **Reporter Ion Cross-Channel Signals in TMT Multiplexing for the Carrier/Reference Strategy;** Paul Stemmer[1]; Nicholas J. Carruthers[1]; Joseph A Caruso[1]; David M. Lubman[2]; Zhijing Tan[2]; *[1]Wayne State University, Detroit, MI; [2]University of Michigan, Ann Arbor, MI*

WP 737 **MRM Based Characterization of the Effect of HIV Infection and Methamphetamine Exposure on Human Monocyte Derived Macrophages;** Sarah C. Zieschang[1]; Shulei Lei[1]; Emma Harwood[1]; Katarzyna Lech[1,2]; Spencer Marshall Jaquet[1]; Brenda Morsey[1]; Howard S. Fox[1]; Pawel Ciborowski[1]; *[1]University of Nebraska Medical Center, Omaha, NE; [2]Faculty of Chemistry, Warsaw University of Technology, Warsaw, Poland*

WP 738 **MS Based Proteomics Reveals Differentially Regulated Proteins in Temozolomide Resistant Glioma;** Milan V. Teraiya[1,2]; Helene Perreault[1]; Vincent C. Chen[3]; *[1]University of Manitoba, Winnipeg, MB; [2]Brandon University (Visiting Student), Brandon, Manitoba; [3]Brandon University, Brandon, Manitoba*

WP 739 **Quantitative Proteomics of Differential Protein Expression in USP24 Depleted Systems;** Joanne Y Chan[1,2]; John Le[2]; Lihua Jiang[1]; Ruiqi Jian[1]; Michael Snyder[1]; Feng Gong[2]; *[1]Stanford University, Stanford, CA; [2]University of Miami Miller School of Medicine, Miami, FL*

WP 740 **Targeted Proteomic Analysis of Small GTPases in Murine Adipogenesis;** Yen-Yu Yang[1]; Ming Huang[2]; Yinsheng Wang[2]; *[1]University of California Riverside, Riverside, CA; [2]University of California, Riverside, Riverside, CA*

WP 741 **A Filter-Assisted Approach for Rapid Proteomic Sample Quality Estimation;** Jair T Montford[1]; Wenjing Peng[1]; Jingfu Zhao[1]; Aiying Yu[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

WP 742 **Proteomic Analysis of Plasma – Sample Preparation and Multiplexing Workflows for Relative Quantitation**; Sergei Snovida[1]; Yen-Chun Lai[2]; Amarjeet Flora[1]; Ryan D. Bomgarden[1]; John C Rogers[1]; *[1]Thermo Fisher Scientific, Rockford, IL; [2]Indiana University School of Medicine, Indianapolis, IN*

WP 743 **Benchtop Instrument for Performing Hands-Free, Standardized Sample Preparation for Quantitative Proteomic Analyses**; Greg A. Foster[1]; Woong Kim[1]; Ryan D. Bomgarden[2]; Suzanne M. Smith[2]; Daniel Lopez-Ferrer[1]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Rockford, IL*

WP 744 **A Standardized Workflow for Tandem Mass Tags™ (TMT™) Based Proteomic Quantification Yields Improved Performance, Reproducible Quantitation, and Throughput Efficiency**; Aaron Robitaille[1]; Ryan D. Bomgarden[2]; Amarjeet Flora[2]; Sergei Snovida[2]; Rosa Viner[1]; Daniel Lopez-Ferrer[1]; Andreas Huhmer[1]; John C Rogers[2]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Thermo Fisher Scientific, Rockford, IL*

SMALL MOLECULES: QUANTITATIVE ANALYSIS
745-769

WP 745 **High-Throughput Quantitative Measurement of Acetylsalicylic Acid, Salicylic Acid and Omeprazole in Human Plasma using LC-MS/MS**; Jingduan Chi[1]; Fumin Li[1]; *[1]PPD Inc, Madison, WI*

WP 746 **Multivariate Approach to On-Line Supercritical Fluid Extraction – Supercritical Fluid Chromatography - Mass Spectrometry Method Development**; Alison P Wicker[1]; Kenichiro Tanaka[2]; Masayuki Nishimura[3]; Vivian Chen[3]; Tairo Ogura[2]; William Hedgepeth[3]; Kevin A. Schug[1]; *[1]University of Texas at Arlington, Arlington, TX; [2]Shimadzu Corporation, Nakagyo-ku, Japan; [3]Shimadzu Scientific Instruments, Inc, Innovation Center, Columbia, MD*

WP 747 **Electrochemistry-Assisted Absolute Quantitation by Mass Spectrometry**; Pengyi Zhao[1]; Hao Chen[1]; *[1]New Jersey Institute of Technology, Newark, NJ*

WP 748 **Development and Validation of a Simple and Rugged LC-MS/MS Method to Measure 17-Desacetyl Norgestimate in Human Plasma**; Nick Peng[1]; Ben Gaboury[1]; Ardeshir Khadang[1]; *[1]Axis Clinicals, Dilworth, MN*

WP 749 **High Throughput MS Testing of APX001A in Rat Tissues**; China Y. Lim[1]; Nidhi Jaiswal[1]; Ben Johnson[1]; Lucie Loukotkova[1]; Robert Mansbach[2]; Karen J. Shaw[2]; Scott Reuschel[1]; Troy Voelker[1]; *[1]Covance, Salt Lake City, UT; [2]Amplyx Pharmaceuticals, San Diego, CA*

WP 750 **Determination of Latanoprost and Latanoprost Free Acid in Plasma by LC-MS/MS Using Electrospray and UniSpray**; Matej Simek[1,2]; Tereza Foglová[1]; Petr Šulc[1]; Martina Hermannová[1]; Vladimír Velebný[1]; *[1]Contipro, Dolni Dobrouc, Czech Republic; [2]Palacký University, Olomouc, Czech Republic*

WP 751 **Overcoming Challenges to Develop a Robust Method for Quantifying Urinary Mono-Hydroxylated Polycyclic Aromatic Hydrocarbons (OH-PAHs) by On-Line SPE-LC-MS**; Yuesong Wang[1]; Erin N. Pittman[1]; Debra A. Trinidad[1]; Hei Sio Ao[1]; Antonia M. Calafat[1]; Julianne C. Botelho[1]; *[1]CDC, Atlanta, GA*

WP 752 **Development and Validation of an Analytical Method for Quantitation of Emtricitabine, Tenofovir, and Efavirenz in Mouse Tissues by UPLC-MS/MS**; Jennifer A. Gilliam[1]; Melanie A. Rehder Silinski [1]; Brenda L. Fletcher[1]; Reshan A. Fernando[1]; Veronica G. Robinson[2]; Suramya Waidyanatha[2]; *[1]RTI International, Research Triangle Park, NC; [2]Division of the National Toxicology Program, NIEHS, Research Triangle Park, NC*

WP 753 **Ultrasensitive Quantification of Fluticasone Propionate and Salmeterol from Human Plasma Using UPLC/MS/MS**; Michael D Jones[1]; Nikunj Tanna[1]; *[1]Waters Corporation, Milford, MA*

WP 754 **Development of a Rapid Method for the Quantification of Fidaxomicin from Biological Samples**; Anthony Haag[1,2]; Kathleen M Hoch[1,2]; Sigmund J Haidacher[1,2]; *[1]Baylor College of Medicine, Houston, TX; [2]Texas Children's Hospital, Houston, Texas*

WP 755 **Analysis of Propylene Glycol in Rat Plasma after Derivatization using Liquid Chromatography Coupled with Tandem Mass Spectrometric Detection (LC-MS/MS)**; Changyu Quang[1]; William C. Nethero[1]; Donald B. Giroux[1]; Liam Moran[1]; Elizabeth A Groeber[1]; *[1]Charles River, Ashland, OH*

WP 756 **Delivery Efficiency of Aerosolized Epoprostenol to the Lung through a Mechanical Ventilator Circuit**; Paul S. Soma[1]; Nicholas J. Wallbillich[1]; Jhaymie L. Cappiello[2]; Gary L. Glish[1]; *[1]University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]Duke University Hospital, Durham, NC*

WP 757 **Trace Level Analysis of Dithiothreitol in Complex Proteins by LC/MS/MS Analysis**; Jeffrey M. Selenka[1]; Christopher G. Ciptadjaya[1]; Thomas Leitzinger[1]; Jie Ding[1]; *[1]PPD, Middleton, WI*

WP 758 **A Rapid and Sensitive LC-MS/MS Method for Quantitative Analysis of GSK-3 Inhibitors in Mouse Plasma**; Ruhan Wei[1]; David Wald[2]; Aimin Zhou[1]; *[1]Cleveland State University, Cleveland, OH; [2]Case Western Reserve University, Cleveland, OH*

WP 759 **Using Labeling Probes and Isotope Tagging for Detection and Quantification of Short Chain Fatty Acids by LCMS in Biological Samples**; Rikard Fristedt; *Chalmers University of Technology, Gothenburg, Sweden*

WP 760 **Investigation of Structure-Dependent Detection Limits for Phthalates, Nitrosamines, Alkylphenols and Aminoglycosides Extracted from Complex Sample Matrix Using LC-MS/MS**; Peijun Tu; *Intertek, Allentown, PA*

WP 761 **Quantification of Tapentadol and Metabolites in Urine by Liquid Chromatography-Mass Spectrometry**; Suraj Saraswat[1]; Kamisha L Johnson-Davis[1,2]; *[1]ARUP Institute for Clinical and Experimental Pathology, Salt Lake City, UT; [2]University of Utah Health Sciences Center, Department of Pathology, Salt Lake City, UT*

WP 762 **Development of a Sensitive and Rugged LC(HILIC)-MS/MS Method for Pantothenic Acid in Human Plasma and Whole Blood Samples**; Xiaodong Zhu[1]; Jingguo Huo[1]; Thomas Lloyd[1]; Edward Wells[1]; *[1]Worldwide Clinical Trials, Austin, TX*

WP 763 **Method Validation for the Determination of Novel Psychoactive Substances in Human Urine by Liquid Chromatography/High Resolution Mass Spectrometry**; Amber Awad[1]; Ana Celia Grenier[1]; Lawrence J Andrade[1]; *[1]Dominion Diagnostics, North Kingstown, RI*

WP 764 **A Fast and Simple Analysis of a Wide Range of Polar Compounds in Spent Media using Ultivo LC/TQ**; Jennifer Cottine Hitchcock[1]; Jordy J. Hsiao[1]; Yanan Yang[1]; *[1]Agilent Technologies, Santa Clara, CA*

WP 765 **Separation Efficiencies of PFP Columns in Reversed Phase Chromatography**; Koji Suzuki[1]; Hiroshi Oikawa[1]; Nozomi Murayama[1]; Hiromi Miyagawa[1]; Masatoshi Akitake[1]; Bruno Ogawa[1]; Natsuki Saotome[1]; Yukio Otsuka[1]; Hideo Matsuoka[1]; Atsushi Sato[1]; *[1]GL Sciences, Saitama, Japan*

WP 766 **Quantitative Variability of Fat-Soluble Vitamins, Hormones, and Mycotoxin Content in Caged, Cage-Free, free-Range, Pasture Raised, and Home Raised chicken eggs**; Jamie L. York[1]; Kevin A. Schug[1]; *[1]The University of Texas at Arlington, Arlington, TX*

WP 767 **LC/MS/MS Analysis for Restricted Chemicals in Textiles**; Tetsuo Tanigawa[1]; Natsuyo Asano[2]; Jun Watanabe[2]; Yin Ling Chew[1]; Jun Xiang Lee[1]; Jie Xing[1]; Zhaoqi Zhan[1]; *[1]Shimadzu (Asia Pacific) Pte Ltd., Singapore, Singapore; [2]Shimadzu Corporation, Nakagyo-ku, Japan*

WP 768 **Modified Mass Barcoded AuNPs Signal Amplification for the Detection of Amphetamines with Laser Desorption Ionization Time-of-Flight Mass Spectrometer**; Liu-ti Wang[1]; He-Hsuan Hsiao[1]; *[1]Department of Chemistry, National Chung Hsing University, Taichung City, Taiwan*

WP 769 **A HILIC-MS Method to Quantitate a Phospholipid Adjuvant for Vaccines**; Bin Deng[1]; Carol Claus[1]; Eric Yang[1]; *[1]Sanofi Pasteur, Toronto, ON*

TOXICOLOGY
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WP 770 **Untargeted Profiling of Toxicologically Relevant Metabolites: Case Study of Reactive Aldehydes**; Loïc Mervant[1,2]; Robin Costantino[3]; Jean-François Martin[3]; Laurent Debrauwer[3]; Françoise Guéraud[2]; Emilien L Jamin[3]; *[1]MetaboHUB-MetaToul, Toulouse, France; [2]Toxalim (Research Centre in Food Toxicology) University of Toulouse, INRA, Toulouse, France; [3]MetaboHUB-MetaToul, Toulouse, France*

WP 771 **Optimization of Collision Cell Potentials for Analysis of Opiates and their Glucuronyl Metabolites in a Triple Quadrupole Mass Spectrometer**; Bennett Kalafut[1]; Jianyun Zhao[1]; Harald Oser[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

WP 772 **Glucuronide Hydrolysis Optimization for Drugs Screening in Urine Using LDTD-MS/MS at 8 seconds per sample**; Serge Auger[1]; Pier-Luc Plante[2]; Jean Lacoursière[1]; Pierre Picard[1]; *[1]Phytronix Technologies, Quebec, QC; [2]Université Laval, Quebec, Quebec*

WP 773 **Quantitative Swab Touch Spray Mass Spectrometry for Oral Fluid Drug Testing**; Nicolas M. Morato[1]; Valentina Pirro[1]; Patrick W. Fedick[1]; Stuart A. Kushon[2]; R. Graham Cooks[1]; *[1]Purdue University, West Lafayette, IN; [2]Neoteryx, Torrence, CA*

WP 774 **Urine Pain Panel Drug Screen for 42 Analytes with Enzyme Hydrolysis and an Internal Hydrolysis Indicator in Each Patient Sample**; Stephen D Merrigan[1]; Gwendolyn A McMillin[1,2]; *[1]ARUP Institute for Clinical and Experimental Pathology, Salt Lake City, UT; [2]University of Utah Health Sciences Center, Department of Pathology, Salt Lake City, UT*

WP 775 **Advancing Forensic DUID Screening with Mass Spectrometry**; Oscar Cabrices[1]; Pierre Negri[2]; Dean Fritch[3]; Melanie Stauffer[3]; Nadine Koenig[3]; Derrick Schollenberger[3]; Jennifer Gilman[3]; Adrian Taylor[4]; *[1]SCIEX, Redwood Shores, CA; [2]SCIEX, Redwood City, CA; [3]Health Network Laboratories, Allentown, PA; [4]SCIEX, Concord, ON*

WP 776 **Streamlining Unknown Screening for Postmortem Analysis**; Adrian Taylor[1]; Oscar Cabrices[2]; Xiang He[2]; Dean Fritch[3]; Nadine Koenig[3]; Melanie Stauffer[3]; Derrick Schollenberger[3]; *[1]SCIEX, Concord, ON; [2]SCIEX, Redwood Shores, CA; [3]Health Network Laboratories, Allentown, PA*

WP 777 **Monitoring the Human Serum Albumin Adductome for Contact Allergens**; Lorena Ndreu[1]; Alister James Cumming[2]; Johan Eriksson[1]; Margareta Törnqvist[1]; Isabella Karlsson[1]; *[1]Department of Analytical Chemistry and Environmental Sciences (ACES), Stockholm University, Stockholm, Sweden; [2]Department of Biochemistry and Biophysics, Stockholm University, Stockholm, Sweden*

WP 778 **Mass Spectrometric Identification and Estrogenic Potential of cyclic Phenone Metabolites Formed in *in vitro* Assays with Fish Liver Slices**; Jose Serrano[1]; Richard C Kolanczyk[2]; Mark A Tapper[2]; Barbara R Sheedy[2]; Tylor J Lahren[2]; Patricia A Kosian[2]; Alena Kubatova[3]; *[1]USEPA.ORD/NHEERL, Duluth, MN; [2]USEPA.ORD/NHEERL, Duluth, Minnesota; [3]University of North Dakota Department of Chemistry, Grand Forks, North Dakota*

WP 779 **UHPLC-nanoESI-MSnMethod for Quantification of DNA Adducts from Meat Carcinogens Implicated in Colorectal Cancer**; Dmitri Konorev[1]; Lihua Yao[1]; Robert Turesky[1]; *[1]Masonic Cancer Center, U of MN, Minneapolis*

WP 780 **Evaluating the Tolerance Mechanism of Zebrafish Embryo to Spermidine Carbon Quantum Dots by Proteomics Analysis**; YuJu Chen[1]; Pang-Hung Hsu[2]; Han-Jia Lin[2]; *[1]National Yang-Ming University, Taipei, Taiwan; [2]National Taiwan Ocean University, Keelung, Taiwan*

WP 781 **Presumptive and Definitive Analysis of Urine Antidepressants by Prelude LX-4 MD™ and Sciex 4500 LC-MS/MS**; Anita Dermartirosian[1]; Edith Shahbol[1]; Karin Thomassian[1]; Shaun Rezaei[1]; Asad Shah[1]; *[1]Quest Diagnostics, Inc., Valencia, CA*

WP 782 **Quantitation of Total Carbamazepine and Carbamazepine Epoxide in Serum/Plasma on HPLC-MS/MS**; Diane Ly[1]; Kamisha L. Johnson-Davis[1,2]; *[1]ARUP Institute for Clinical and Experimental Pathology, Salt Lake City, UT; [2]University of Utah Health Sciences Center, Department of Pathology, Salt Lake City, UT*

WP 783 **Toxicological and Biochemical Changes Induced by Sub-Acute Exposure of Wistar Rats to Silver Nanoparticles using Soft Landing Ion Mobility Instrument**; Subhayu Nayek[1]; Guido F. Verbeck[1]; *[1]University of North Texas, Denton, TX*

WP 784 **Small Molecules Automated Extraction from Human Breast Milk Using the Extrahera and the EVOLUTE Express CX Prior to LC-MS/MS Analysis**; Mohamed Youssef[1]; Stephanie Marin[1]; Jillian Neifeld[1]; Jeremy Smith[1]; Mario Merida[1]; Elena Gairloch[1]; *[1]Biotage, Charlotte, NC*

WP 785 **Quantitative Proteomic Analysis of Cardiac Endothelial Cells Treated with Doxorubicin**; Xinzhu Pu[1]; Steve Nick[1,2]; Matthew Turner[1]; Laura Bond[1]; Kenneth Cornell[1]; *[1]Boise State University, Boise, ID; [2]University of Arizona, Tucson, AZ*

WP 786 **Effects of DDE/Dieldrin on the Steroid Hormone Profile in Largemouth Bass (Micropterus Salmoides) Plasma**; Mohammad-Zaman Nouri[1]; Kevin J. Kroll[1]; Nancy D. Denslow[1]; *[1]Department of Physiological Sciences and Center for Environmental and Human Toxicology, University of Florida, Gainesville, FL*

WP 787 **Alternative Forensic Matrices: Evaluation of Simplified Workflow for Drugs of Abuse Extraction from Nail Samples Prior to LC-MS/MS Analysis**; Katie-Jo Teehan[1]; Lee Williams[1]; Rhys Jones[1]; Geoff Davies[1]; Adam Senior[1]; Helen Lodder[1]; Alan Edgington[1]; Steve Jordan[1]; Claire Desbrow[1]; Paul Roberts[1]; *[1]Biotage GB Limited, Cardiff, United Kingdom*

WP 788 **Using a LC/MSD XT Single Quadrupole and HILIC-Z Column for Sensitive and Reliable Detection of Potential Genotoxic Impurities**; Patrick M Batoon[1]; Kyle Covert[2]; *[1]Agilent Technologies Inc., Santa Clara, CA; [2]Agilent Technologies, Inc., Santa Clara, CA*

WP 789 **Method Validation for Trace Phentermine in the Presence of High Methylamphetamine Concentration and Other Analytes in Human Urine by LC-MS/MS**; Jianmei Wang[1]; Jeremy Delao[1]; *[1]Spectrum Diagnostic Laboratories, Arlington, TX*

Set up all Thursday posters
7:00 - 8:00 am

Odd-numbered posters present
10:30 - 11:30 am PLUS 12:30 – 2:30 pm

Even-numbered posters present
10:30 am - 12:30 pm PLUS 1:30 – 2:30 pm

Remove all Thursday posters
2:30 - 3:00 pm

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Ambient Ionization: Fundamentals and Instrumentation 033-059
Carbohydrates II 060-085
Data-Dependent Acquisition 086-092
Data-Independent Acquisition 093-111
Disease Biomarkers II 112-130
Drug Discovery/DMPK/ADME II 131-152
Drug Metabolism: Quantitative Analysis 153-159
Elemental Analysis: ICP/MS 160-175
Elemental Analysis: Isotope Ratio MS 176
Exposomics Methodologies and Research Results 177-181
Food "omics" MS Characterization of Food and Nutritional Supplements II 182-203
Glycoproteins II 204-224
Imaging MS: Disease Markers II 225-242
Imaging MS: Method Development II 243-263
Informatics: General, SRM, and DIA 264-272
Ion Mobility: Applications III 273-294
Ion Mobility: Fundamentals 295-320
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LC/MS: Chromatography and Software II 332-352
LC/MS: Sample Preparation II 353-377
Lipids: ID and Structural Analysis 378-404
MALDI: Applications 405-417
MALDI: Fundamentals and Instrumentation 418-421
MALDI: Sample Preparation 422-430
Metabolomics: Clinical Applications 431-449
Metabolomics: General II 450-478
Metabolomics: Sample Preparation 479-482
Metabolomics: Untargeted Metabolite Profiling III 483-512
Microorganisms: Identification and Characterization 513-540
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Nanoscale and Microfluidic Separations and MS 549-566
Natural Products 567-589
Nucleic Acids and Oligonucleotides II 590-611
Peptides: Fragmentation Mechanisms 612-617
Proteins: Complexes/Non-covalent Interactions II 618-635
Proteins: Conformation Analysis and Structural Biology 636-653
Proteins: General and Membrane 654-673
Proteins: PTMs II 674-697
Proteomics: New Approaches II 698-724
Proteomics: Quantitative IV 725-749
Small Molecules: Quantitative Analysis II 750-777

AMBIENT IONIZATION: APPLICATIONS II
001-032

ThP 001 **Molecular Profiling of Cyanobacteria under Environmental Stimuli Using Laser Ablation Electrospray Ionization Coupled with Ion Mobility Separation Mass Spectrometry**; Gessica Vasconcelos[1]; Sylwia A Stopka[2]; Boniek G Vaz[1]; Akos Vertes[2]; *[1]Federal University of Goias, Goiania, Brazil; [2]George Washington University, Washington, DC*

ThP 002 **Accelerated Energetic Syntheses through the Use of Confined Volume Systems Generated by Ambient Ionization Sources**; Patrick W Fedick; *Naval Air Warfare Center, Weapons Division, Research Department, Chemistry Division, China Lake, CA*

ThP 003 **Highly Sensitive and Rapid Screening for Pesticides using Direct Analysis in Real Time Triple Quadrupole Mass Spectrometry**; He Cui[1]; Yongyi Jiang[2]; Kerry Song[3]; Xiuzhen Yin[1,4]; Tingting Han[2]; Jiale Xu[3]; Xiaokun Duan[3]; Charles C. Liu[3]; *[1]Qingdao Customs District, Qingdao, China; [2]Qingdao Future Test, Qingdao, China; [3]ASPEC Technologies, Beijing, China; [4]Qingdao University of Science and Technology, Qingdao, China*

ThP 004 **Detection of Ricin and Abrin Toxin by Laboratory-Based and Portable Direct Analysis in Real-Time Mass Spectrometry (DART-MS)**; Jennifer W Sekowski[1]; Debora Van Der Riet-van Oeveren[2]; Ad De Jong[2]; Alex Fidder[2]; Paul S Demond[1]; Jacquelyn V Harris[1]; Daan Noort[2]; *[1]U.S. Army RDECOM Chemical & Biological Center, Aberdeen Proving Ground, MD; [2]The Netherlands Organization, Rijswijk, Netherlands*

ThP 005 **Solvent-Assisted Paper Spray Ionization Mass Spectrometry (SAPSI-MS) for the Analysis of Biomolecules and Biofluids**; Alessandro Quaranta[1]; Nicolò Riboni[1]; Hitesh V Motwani[1]; Nicklas Österlund[1]; Astrid Gräslund[1]; Federica Bianchi[2]; Leopold L Ilag[1]; *[1]Stockholm University, Stockholm, Sweden; [2]University of Parma, Parma, Italy*

ThP 006 **Improved Sensitivity for Saccharides *via* In-Source Derivatization Using Coaxial Contained Electrospray Mass Spectrometry**; Derik R. Heiss[1,2]; Abraham K. Badu-Tawiah[3]; *[1]The Ohio State University, Columbus, OH; [2]Battelle Memorial Institute, Columbus, OH; [3]The Ohio State University, Columbus, OH*

ThP 007 **Cross-Continental, Multisite Round Robin REIMS Study for the Evaluation of REIMS Fundamentals and Technology**; Julia Balog[1]; Pierre-Maxence Vaysse[2]; Tiffany Porta Siegel[2]; Martin Kaufmann[3]; Ala Amgheib[4]; Viktoria Varga[1]; Andras Marton[1]; Steven D Pringle[5]; John Rudan[3]; Ron M. A. Heeren[2]; Zoltan Takats[4]; *[1]Waters Research Center, Budapest, Hungary; [2]Maastricht Multimodal Molecular Imaging (M4I) Institute, Division of Imaging Mass Spectrometry, Maastricht, Netherlands; [3]Queen's University, Kingston, ON; [4]Imperial College, London, United Kingdom; [5]Waters Corporation, Wilmslow, United Kingdom*

ThP 008 **Molecular Characterization of Terminal Structures for Polycarbonates Using a Thermal Desorption/Pyrolysis DART-MS**; Kenichi Yoshizawa[1]; Chikako Takei[1]; Sayaka Nakamura[2]; Hiroaki Sato[2]; *[1]BioChromato, Inc., Fujisawa, Japan; [2]National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan*

ThP 009 **Improved Rapid Untargeted Screening Method for Veterinary Drug Residues in Animal Tissues Using Liquid Microjunction Surface Sampling Probe Mass Spectrometry**; Laura Burns[1]; David J. Borts[1,2]; *[1]Interdepartmental Toxicology Program, Iowa State University, Ames, Iowa; [2]Department of Veterinary Diagnostic & Production Animal Medicine, Iowa State University, Ames, IA*

ThP 010 **Flavor release monitoring using direct analysis in real-time mass spectrometry on differentiate with respect to time**; Motoshi Sakakura[1]; Teruhisa Shiota[1]; Takehito Sagawa[2]; *[1]AMR, Inc., Tokyo, Japan; [2]S&B foods Inc., Tokyo, Japan*

ThP 011 **Revealing Photo-Thermal Stability of Pharmaceuticals and the Degradation Mechanism by Microwave Plasma Torch Mass Spectrometry**; Shuanglong Wang[1]; Wei Liu[1]; Huanwen Chen[1]; *[1]East China University of Technology, Nanchang, China*

ThP 012 **Electroextraction (EE) Coupled with Paper Spray Mass Spectrometry (PS-MS) for Selective and Sensitive Analyses of Target Analytes in Complex Samples**; Rodinei Augusti[1]; Victoria Silva Amador[1]; Juliane Soares Moreira[1]; Denise Versiane Monteiro de Sousa[1]; Ricardo Mathias Orlando[1]; *[1]Federal University of Minas Gerais, Belo Horizonte, Brazil*

ThP 013 **A Robust, Long-Lasting Microspray Metal Emitter with Nanospray Sensitivity for Proteomics**; Sau Lan Staats[1]; Anna Stoltzfus[1]; Andris Suna[1]; *[1]Phoenix S & T, Inc, Chadds Ford, PA*

ThP 014 **Quantitative Analysis of Linezolid in Human Plasma by DART-MS and its Application to a Pharmacokinetic Study**; Lei Yin[1,2,3]; Yixuan Feng[1,2]; Jin Tong[1,2]; Zhiqiong Guo[1,2]; Yuyao Zhang[1,2]; Xiaokun Duan[4]; Lifeng Xu[4]; Charles C. Liu[4]; Jingkai Gu[*1,2]; *[1]Jilin University, Changchun, China; [2]Beijing Institute of Modern Drug Metabolism, Beijing, China; [3]University of Arizona, Tucson, AZ; [4]ASPEC Technologies, Beijing, China*

ThP 015 **Reaction Acceleration at the Surface of Droplets**; Yangjie Li[1]; Zhenwei Wei[1]; Yong Liu[2]; R. Graham Cooks[1]; *[1]Department of Chemistry, Purdue University, West Lafayette, IN; [2]Merck & Co., Inc., Rahway, NJ*

ThP 016 **A Comparative Profiling of DHA-rich Oil Products by DESI and DART Mass Spectrometry**; Kerry Song[1]; Jiale Xu[1]; Wen Zhou[2]; Jiang Zhou[2]; Wei Chen[1]; Xiaokun Duan[1]; Charles C. Liu[1]; *[1]ASPEC Technologies, Beijing, China; [2]Peking University, Beijing, China*

ThP 017 **Repeatability and Practicality of PESI/MS/MS-Based *in vivo* Real-Time Monitoring System for Hepatic/Brain Metabolites in Living Mice**; Kei Zaitsu[1,2]; Yumi Hayashi[1,3]; Tasuku Murata[4]; Kazumi Yokota[4]; Tomomi Ohara[2]; Hitoshi Tsuchihashi[2]; Akira Ishii[2]; Koretsugu Ogata[4]; Hiroshi Taninata[4]; *[1]In Vivo Real-Time Omics Laboratory, Institute for Advanced Research, Nagoya University, Nagoya, Japan; [2]Department of Legal Medicine and Bioethics, Nagoya University Graduate School of Medicine, Nagoya, Japan; [3]Pathophysiological Laboratory Sciences, Department of Radiological and Medical Laboratory Sciences, Nagoya University Graduate School of Medicine, Nagoya, Japan; [4]Shimadzu Corporation, Kyoto, Japan*

ThP 018 **Using Rapid Evaporative Ionisation Mass Spectrometry (REIMS) to Improve Efficiency and Add Capability in Pharmaceutical R&D**; Paul Abu-Rabie; *GSK R&D, Stevenage, United Kingdom*

ThP 019 **Pre-Concentration and a Special Scan Function for More Sensitive and Stable Ambient Ionization Mass Spectrometry**; Taoqing Wang[1]; Linfan Li[2]; Mengtian Li[1]; Huishan Li[1]; Jae C Schwartz[2]; Anyin Li[1]; Nicolas Heath[1]; *[1]University of New Hampshire, Durham, NH; [2]Thermo Fisher Scientific, San Jose, CA*

ThP 020 **Coated Blade Spray–High-Resolution Mass Spectrometry: A Versatile Tool for Sample Profiling and Screening of Controlled Substances in Complex Matrices**; German Augusto Gómez-ríos[1]; Robert Cody[2]; Nathaly Reyes-garcés[1]; Frances Carroll[1]; Gary Stidsen[1]; David Bell[1]; *[1]Restek Corporation, Bellefonte, PA; [2]JEOL USA, Inc., Peabody, MA*

ThP 021 **Extractable Analysis of Heart Stem Using HPLC Q-Tof Mass Spectrometry Coupled with High Resolution Database and Library**; Chang Jiang; *, Chengdu, China*

ThP 022 **Ion-Neutral Complex Mediated Benzyl Cation Transfer and Proton Transfer of Protonated Benzyl Phenyl Sulfonein the Gas Phase**; Yin Qi; *Zhejiang University, Hangzhou, China*

ThP 023 **Rapid Characterization of Saponins in Ginseng Species Roots by Liquid Extraction Surface Analysis Mass Spectrometry**; Mei Tian[1]; Yuangui Yang[1]; Linnan Li[1]; Li Yang[1,2]; Xiaokun Duan[3]; Kerry Song[3]; Shujie Zou[3]; Echo Jia[3]; Charles.C Liu[3]; Zhengtao Wang[1,2]; *[1]Shanghai University of Traditional Chinese Medicine, Shanghai, China; [2]Shanghai R&D Center for Standardization of Chinese Medicines, Shanghai, China; [3]ASPEC Technologies, Beijing, China*

ThP 024 **Analysis of Immunosuppressant Drugs directly from Whole Blood using PaperSpray Technology**; Cornelia Leonie Boeser[1]; Neloni R. Wijeratne[1]; Mary L. Blackburn[1]; *[1]Thermo Fisher Scientific, San Jose, CA*

ThP 025 **Sticky Paper Spray Ionization for Analysis of Powdered Analyte Grains**; Praneeth Hettikankanange[1]; Grant Klingler[1]; Mason Laikupu[1]; Daniel Austin[1]; *[1]Brigham Young University, Provo, UT*

ThP 026 **Mechanistic Study of Organometallic Reactions by On-line Mass Spectrometry Monitoring System**; Xin Yan; *Texas A&M University, College Station, TX*

ThP 027 **Strain-Level Differentiation of Bacteria by Paper Spray Mass Spectrometry**; Casey A. Chamberlain[1]; Vanessa Y. Rubio[1]; Timothy J. Garrett[1]; *[1]University of Florida, Gainesville, FL*

ThP 028 **Areca Alkaloids Measured from Buccal Cells Using DART-MS Serve as Accurate Biomarkers for Betel Nut Chewing**; Adrian Franke[1]; Laura Biggs[2]; Joanne Y. Yew[3]; Jennifer F Lai[4]; *[1]Univ of Hawaii Cancer Ctr, Honolulu, HI; [2]University of Guam, Mangilao, Guam; [3]Pacific Biosciences Research Center, University of Hawaii, Honolulu, hawaii; [4]University of hawaii Cancer Center, Honolulu, Hawaii*

ThP 029 **Microdroplet Fusion Chemistry for Charge State Reduction in Synthetic and Biological Polymers via Bipolar Dual Spray**; John R Stutzman[1]; Ryan M Bain[1]; Sebastian Hagenoff[2]; William Hunter Woodward[1]; John P O'Brien[3]; Michael Lesniak[1]; *[1]The Dow Chemical Company, Midland, MI; [2]The Dow Chemical Company, Stade, Germany; [3]The Dow Chemical Company, Lake Jackson, TX*

ThP 030 **Application of the Micro Flow Ion Source with Cartridge Columns for Fast LC-MS/MS Analysis of Vitamin D Metabolites**; Tomasz Bienkowski[1]; Michał Szumski[1,2]; Irmina Tomaszewska[1]; Konrad Piotr Kowalski[1]; Przemysław Kalicki[1]; Michał Książkiewicz[1]; *[1]MS Ekspert Sp. z o.o, Gdańsk, Poland; [2]Nicolaus Copernicus University, Torun, Poland*

ThP 031 **Quality Control Aspects of the REIMS Technology**; Andras Denes Marton[1]; Richard Schäffer[1]; Viktoria Varga[1]; Tamas Karancsi[1]; Lajos Godorhazy[1]; Steven D Pringle[2]; Julia Balog[1,3]; *[1]Waters Research Center, Budapest, Hungary; [2]Waters Corporation, Wilmslow, United Kingdom; [3]Imperial College, London, United Kingdom*

ThP 032 **SpiderMass Real-Time, Mini Invasive Analysis of Cancer: Towards *in vivo* Molecular Diagnostics of the Future**; Nina Ogrinc[1]; Philippe Saudemont[1]; Yves-Marie Robin[2]; Julia Balog[3]; Dominique Tierny[4]; Jean-Pascal Gimeno[1]; Zoltan Takats[5]; Michel Salzet[1]; Isabelle Fournier[1]; *[1]PRISM Inserm U1192 - University of Lille, Villeneuve D'ascq Cedex, France; [2]Pathology Department, Centre Oscar Lambret, Lille, France; [3]Waters Research Center, Budapest, Hungary; [4]OCR, Villeneuve d'Ascq, France; [5]Imperial College London, London, United Kingdom*

AMBIENT IONIZATION: FUNDAMENTALS AND INSTRUMENTATION
033-059

ThP 033 **Unique Ion/Molecule Chemistry of N-Alkanes in the Flowing Atmospheric Pressure Afterglow Ionization Source;** Brian Molnar[1]; Sunil P Badal[1]; Jacob T Shelley[1]; *[1]Rensselaer Polytechnic Institute, Troy, NY*

ThP 034 **Visualization of Charged Droplets – Ambient Gas Interactions and Entrainment Flows in Nanoelectrospray;** Joel Chapman[1]; Peter Kottke[1]; Andrei Fedorov[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

ThP 035 **Wire Desorption-Glow Discharge/Electrospray Ionization/Mass Spectrometry for Rapid Characterization of Compounds with a Broad Range of Polarity and Boiling Point;** Yuanlong Wang[1]; Junsheng Zhang[1]; Lin Liu[1]; Liping Huang[1]; Jentaie Shiea[2]; Wenjian Sun[1]; *[1]Shimadzu Research laboratory (Shanghai) Co. Ltd., Shanghai, China; [2]Department of Chemistry, National Sun Yat-sen University, Kaohsiung, Taiwan*

ThP 036 **Direct Mass Spectrometry Analysis Using In-Capillary Dicationic Ionic Liquid-Based *in situ* Dispersive Liquid-Liquid Microextraction and Sonic-Spray Ionization;** Yueguang Lv[1]; Qiang Ma[1]; *[1]Chinese Academy of Inspection and Quarantine, Beijing, China*

ThP 037 **The Effects of Gas Flows and Discharge Pulse on Explosives Detection Using a Dielectric Barrier Discharge Ionization Source;** Vadym Berkout; *Smiths Detection, Edgewood, MD*

ThP 038 **Atmospheric Pressure Dark-Current Argon Discharge Ionization with Comparable Performance to Direct Analysis in Real Time Mass Spectrometry;** Teruhisa Shiota[1]; Kanako Sekimoto[2]; Motoshi Sakakura[1]; Mitsuo Takayama[2]; *[1]AMR, Inc., Tokyo, Japan; [2]Yokohama City University, Yokohama, Japan*

ThP 039 **Sampling and Ionization Process in Scanning Probe Electrospray Ionization;** Yoichi Otsuka[1]; Bui Kamihoriuchi[1]; Aya Takeuchi[1]; Futoshi Iwata[2]; Takuya Matsumoto[1]; *[1]Osaka University, Toyonaka, Japan; [2]Shizuoka University, Hamamatsu, Japan*

ThP 040 **Inlet Ionization for High Speed Mass Spectrometry;** Eilen Inutan[1,2]; Chuping Lee[1]; Eric Davis[1]; Georgios Makris[1]; Frank Yenchick[1]; Robert Roose[1]; Sarah Trimpin[1,3]; *[1]Wayne State University, Detroit, MI; [2]MSU-Iligan Institute of Technology, Iligan City, Philippines; [3]Cardiovascular Research Institute, Wayne State University School of Medicine, Detroit, MI*

ThP 041 **Surface Acoustic Wave Nebulization (SAWN) and Charge Independent Nano Electromechanical Mass Sensing (NEMS-MS) of Multi Mega-Dalton Particles;** Szu-Hsueh Lai[1]; Bogdan Vysotskyi[2]; Luis A Cubero Montealegre[2]; Martial Defoort[2]; Kavya Clement[1]; Mohammad Abdul Halim[1]; Sergio Dominguez-Medina[1]; Sebastien Hentz[2]; Christophe Masselon[1]; *[1]Univ. Grenoble Alpes, CEA, Inserm, BIG-BGE, Grenoble, France; [2]Univ. Grenoble Alpes, CEA, LETI, Grenoble, France*

ThP 042 **An Optimized Jet Nebulization Geometry for LCMS;** Chuck Jolliffe[1]; Harikrishnan Sukumar[1]; Marius Radu[1]; Reza Javahery[1]; *[1]PerkinElmer Inc., Woodbridge, ON*

ThP 043 **Fast Screening of Pesticides in Foods and Agricultural Products with Probe Electrospray Ionization (PESI) Tandem Mass Spectrometry;** Zhenhe Chen[1]; Satoshi Yamaki[1]; Jing Dong[1]; Yuki Hashi[2]; Naoki Hamada[1]; *[1]Shimadzu (China) Co., LTD., Beijing, China; [2]Shimadzu (China) Co.,LTD., Shanghai, China*

ThP 044 **Liquid Ionization with High-Repetition Rate µJ-Laser-Induced Airborne Plasma for Direct Mass-Spectrometric Analysis;** Yi You[1]; Andreas Bierstedt[1]; Sebastian van Wasen[1]; Gaby Bosc-Bierne[1]; Michael G. Weller[1]; Jens Riedel[1]; *[1]Federal Institute for Materials Research and Testing (BAM), Berlin, Germany*

ThP 045 **Solvent Assisted Surface Probe-Nanoelectrospray: A Modular Liquid-Extraction Based Tool for Combined Top-Down & Bottom-Up Proteomic Surface Analysis;** Raul Villacob[1]; Luke T. Richardson[1]; Matthew Mulloy[1]; Touradj Solouki[1]; *[1]Baylor University, Waco, TX*

ThP 046 **Laser Desorption REIMS – the Fundamentals and How they Dictate Applications and Automation;** Emrys A Jones[1]; Daniel Simon[2]; Tamas Karancsi[2]; Danielle McDougall[3]; Csaba Hajdu[2]; Richard Schaffer[2]; Julia Balog[2]; Steven D Pringle[4]; Zoltan Takats[5]; *[1]Waters, Wilmslow, United Kingdom; [2]Waters Research Center Kft., Budapest, Hungary; [3]Manchester Institute of Biotechnology, University of Manchester, United Kingdom; [4]Waters Corporation, Wilmslow, United Kingdom; [5]Imperial College, London, United Kingdom*

ThP 047 **Systematic CFD Study of Gas Transport in a Desorption Cell Coupling AFM and AP MS in a Multimodal Imaging Platform;** Matthias Lorenz[1]; Ryan Wagner[2]; Roger Proksch[2]; Olga S Ovchinnikova[3]; *[1]University of Tennessee / Oak Ridge National Laboratory, Oak Ridge, TN; [2]Oxford Instruments, Santa Barbara, CA; [3]Oak Ridge National Laboratory, Oak Ridge, TN*

ThP 048 **An Interface for Reproducible, Multi-shot Direct Analysis of Solid-phase Microextraction Samples;** G. Asher Newsome[1]; Alba Alvarez-Martin[1]; Gwénaëlle Kavich[1]; *[1]Smithsonian Institution Museum Conservation Institute, Suitland, MD*

ThP 049 **Internal Energy Deposition in Infrared Matrix-Assisted Laser Desorption Electrospray Ionization with and without the Use of Ice as a Matrix;** Angi Tu[1]; David C. Muddiman[1,2]; *[1]FTMS Laboratory for Human Health Research, Department of Chemistry, North Carolina State University, Raleigh, NC; [2]Molecular Education, Technology, and Research Innovation Center (METRIC), North Carolina State University, Raleigh, NC*

ThP 050 **Two-Laser Ablation Electrospray Ionization Mass Spectrometry;** Kelcey B. Hines[1]; Remilekun O. Lawal[1]; Fabrizio Donnarumma[1]; Kermit K. Murray[1]; *[1]Louisiana State University, Baton Rouge, LA*

ThP 051 ***In vivo* Analysis of Plant Sap by Direct Sampling and Capillary Microsampling Electrospray Ionization Mass Spectrometry;** Tina Tran[1]; Laith Z. Samarah[1]; Akos Vertes[1]; *[1]George Washington University, Washington, DC*

ThP 052 **Key Factors Influencing Nano-Electrospray Ionization Efficiency of Tryptic Peptides from Fused Silica Emitters During Reversed-Phase Liquid Chromatography Separations;** Joshua A Silveira[1]; Gary Schultz[2]; Wei Wei[3]; Aran Paulus[3]; Eloy R. Wouters[3]; *[1]Thermo Fisher Scientific, San Jose, CA; [2]Munson Technology, Ithaca, NY; [3]Thermo Fisher Scientific, San Jose, CA*

ThP 053 **The Effect of High Mass Resolving Power by Involving Sample Morphology in Linear TOF;** Yi-Hong Cai; *Genomics Research Center Academia Sinica, Taipei, Taiwan*

ThP 054 **Characterization of a Novel Plasma-Ionization Source for Real-Time Breath Analysis;** Christopher Gongar[1]; Michael Wei[1]; Robin H.J Kemperman[1]; Richard A. Yost[1]; *[1]University of Florida, Gainesville, FL*

ThP 055 **Reactions and Fragmentation in a Microwave Plasma Jet Ambient Ionization Source;** Kenyon Evans-Nguyen[1]; Abigail Smola[1]; Kayla M Whitehouse[1]; Tiffany Matyja[1]; Micheala Le Gendre[1]; *[1]University of Tampa, Tampa, FL*

ThP 056 **Strategies to Improve Protein Analysis by Desorption Electrospray Ionization;** Andre Venter[1]; Elahe Honarvar[1]; Roshan Javanshad[1]; Tara Maser[1]; Frank Martin Beranek[1]; *[1]Western Michigan University, Kalamazoo, MI*

ThP 057 **Development of a Cryo-Stage for LESA Mass Spectrometry – Towards Truly Native Surface Sampling of Proteins;** Bin Yan[1]; Adam J. Taylor[1]; Josephine Bunch[1,2];

[1]National Physical Laboratory, Teddington, United Kingdom; [2]Imperial College, London, United Kingdom

ThP 058 **Trace Level Detection of Gas Impurities Using Atmospheric Pressure Ionization Mass Spectrometry**; Gregory Thier[1]; Luke Kephart[1]; Brian Regel[1]; [1]Extrel CMS, Pittsburgh, PA

ThP 059 **Investigation of Gas Flow Effects and Space Charge in Atmospheric Pressure Interfaces**; Philipp Krah[1]; Laurent Bernier[1]; Stephan Rauschenbach[2]; Julius Reiss[1]; [1]Technical University Berlin, Berlin, Germany; [2]University of Oxford, Oxford, United Kingdom

CARBOHYDRATES II
060-085

ThP 060 **High-Throughput Clinical Glycomics with Ultra High Resolution MALDI-FTICR-MS Reveals Pancreatic Cancer Disease Signatures**; Gerda C.M. Vreeker[1]; Randa g.h. Sawires[1]; Simone Nicolardi[1]; Marco R. Bladergroen[1]; Jan Nouta[1]; Wilma E. Mesker[1]; Yuri E.M. van der Burgt[1]; Rob A.E.M. Tollenaar[1]; Manfred Wuhrer[1]; [1]Leiden University Medical Center, Leiden, Netherlands

ThP 061 **Automatically Glycan Structural Determination with Logically Derived Sequence Tandem Mass Spectrometry**; Chi-kung Ni[1]; Shih-Pei Huang[1]; Chia Yen Liew[1]; Hsu-Chen Hsu[1]; [1]Academia Sinica, Taipei, Taiwan

ThP 062 **Discrimination of Glycan Epimers *via* Generation of Unique Parent-Structure-Dependent Product Ions by Free Radical Chemistry and Mass Spectrometry**; Jinshan Gao[1]; Kimberly Fabijanczuk[1]; Kaylee Gaspar[1]; Rayan Murtada[1]; [1]Montclair State University, Montcalir, NJ

ThP 063 **Laser Induced Fluorescence Imaging of the Electrospray for Quantitative N-Glycosylation Analysis of Monoclonal Antibodies by Capillary Electrophoresis – Mass Spectrometry**; Andras Guttman; Sciex, Brea, CA

ThP 064 **A Multi-Dimensional HPLC-MS Method for Heparin/ Heparan Sulfate Oligosaccharide Fraction**; Hao Liu[1]; Apoorva Joshi[2]; Pradeep Chopra[2]; Geert-Jan Boons[2,3]; Joshua S Sharp[4]; [1]University of Mississippi, Oxford, MS; [2]University of Georgia, Athens, GA; [3]Utrecht Univeristy, Utrecht, Netherlands; [4]Univerisity of Mississippi, Oxford, MS

ThP 065 **Structure Modeling of Isomeric Ions of Pyridinylboronic Esters of Momo-, Di- and Oligosaccharides from IMS Q-TOF and Tandem Mass Spectrometry**; Jun J Hu[1]; Qidi Wu[1]; Chengyi Xie[1]; [1]Ningbo University, Ningbo, China

ThP 066 **Development of a Multiplatform Mass Spectrometry-Based Workflow for the In-Depth Structural Elucidation of Oligosaccharides and Polysaccharides**; Juan J Castillo[1]; Ace G Galermo[2]; Matthew J Amicucci[3]; Eshani Nandita[3]; Carlito B Lebrilla[3]; [1]University of Davis, Davis, CA; [2]Univerisity of California, Davis, Davis, CA; [3]UC Davis, Davis, CA

ThP 067 **Detailed Glycosylation Analysis: Leukemic KG1a Cells as a Case Study Using Sequential Mass Spectrometry**; David Ashline[1]; Vernon Reinhold[1]; [1]University of New Hampshire, Durham, NH

ThP 068 **Definitive Structural Assignment of Isomeric Glycans by Trapped Ion Mobility-Electronic Excitation Dissociation Tandem Mass Spectrometry**; Juan Wei[1]; Yang Tang[1]; Mark E. Ridgeway[2]; Pengyu Hong[3]; Catherine E. Costello[1]; Cheng Lin[1]; [1]Boston University, Boston, MA; [2]Bruker Daltonics Inc., Billerica, MA; [3]Brandeis University, Waltham, MA

ThP 069 **Automated Identification and Quantitation of 2-AA Derivatized N-Glycans from Infliximab Using UHPLC-Orbitrap-MS Analysis with SimGlycan Software**; Ningombam Sanjib Meitei[1,2]; Himani Gupta[2]; Arun Apte[1]; Phil Widdowson[3]; Silvia Millán[4]; Sara Carillo[4]; Jonathan Bones[4]; Rowan Moore[3]; [1]PREMIER Biosoft, Palo Alto, CA; [2]PREMIER Biosoft, Indore, India; [3]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom; [4]National Institute for Bioprocessing Research and Training, Dublin, Ireland

ThP 070 **Characterization of Glycan Isomers Using Magnetic Carbon Nanoparticles as a MALDI Co-Matrix**; Alireza Banazadeh[1]; Mona Goli[1]; Wenjing Peng[1]; Reed Nieman[1]; Hans Lischka[1]; Yehia Mechref[1]; [1]Texas Tech University, Lubbock, TX

ThP 071 **Isomeric Linkage Determination of Sialic acid on O-Glycopeptides Using O-Protease and LC-MS/MS**; Jieqiang Zhong[1]; Yifan Huang[1]; Wenjing Peng[1]; Yehia Mechref[1]; [1]Texas Tech University, Lubbock

ThP 072 **Deciphering Key Protein Binding Elements within Short- and Medium-Length Heparin Oligomers Using Multidimensional Chromatography Followed by MS Analysis**; Cedric Bobst[1]; Igor A. Kaltashov[1]; [1]University of Massachusetts Amherst, Amherst, MA

ThP 073 **Analysis of the CHO-S Glycocalyx *via* Electrospray Ionization with Tandem Mass Spectrometry**; Amanda J Pearson[1]; Elyssia S. Gallagher[2]; [1]Baylor Univeristy, Waco, TX; [2]Baylor University, Waco

ThP 074 **A Novel Approach Coupling Electrophoresis with Mass Spectrometry for Identification and Characterization of Multicomponent Glycosaminoglycan Drugs**; Anran Sheng[1]; Xiaohui Xu[1]; Lianli Chi[1]; [1]Shandong university, Qingdao, China

ThP 075 **Simultaneous Determination of 18 Monosaccharide Using High Performance Anion-Exchange Chromatography Coupled with Pulsed Amperometric Detection and Tandem Mass Spectrometry**; Feng Feng[1]; Feng Zhang[1]; [1]Institute of Food Safety, Chinese Academy of Inspection and Quarantine, Beijing, China

ThP 076 **Precise Sequencing of Glycosaminoglycan Tetrasaccharides by Reversed Phase Ion Pairing LC/MS and MSn Spectra Matching**; Qing Guo[1]; Vernon Reinhold[1]; [1]University of New Hampshire, Durham, NH

ThP 077 **LC-MS/MS Approach for the Exploration of Glycosylation as a Gatekeeper for Successful Xeno Transplantation**; Myung Jin Oh[1,2]; Nari Seo[1,2]; Jaekyoung Ko[1,2]; Jinyoung Park[1,2]; Xi-jun Yin[3]; Jjin-dan Kang[3]; Hyun Joo An[1,2]; [1]Chungnam national university, Daejeon, South Korea; [2]Asia-Pacific Glycomics Reference Site, Daejeon, South Korea; [3]Yanbian University, Yanji, China

ThP 078 **GlyLipSILC – Glycolipid Stable Isotope Labeling in Cell Cultures**; Andrew Cho[1]; Wenjing Peng[1]; Yifan Huang[1]; Yehia Mechref[1]; [1]Texas Tech University, Lubbock, TX

ThP 079 **Investigation of Ganglioside Isomers to Reveal the Biological Mechanism of Breast Cancer Brain Metastasis Using Nano-ZIC-HILIC-LC-MS**; Yifan Huang[1]; Jieqiang Zhong[1]; Wenjing Peng[1]; Yehia Mechref[1]; [1]Texas Tech University, Lubbock, TX

ThP 080 **Relative Quantification of Glycans in Yeast Using Metabolic Isotope Labeling with Isotopic Glucose by Mass Spectrometry**; Jae-min Lim[1]; Ji-yeon Kim[2]; Soo-hyun Choi[2]; [1]Changwon National University, Changwon, South Korea; [2]Changwon National University, Changwon, South Korea

ThP 081 **Post-Column Chiral Addition Method for the Separation and Resolution of Common Monosaccharides**; Zachary Wooke[1]; Gabe Nagy[1]; Lauren Barnes[1]; Matthew Laing[1]; Nicola L. B. Pohl[1]; [1]Indiana University Bloomington, Bloomington, IN

ThP 082 **Multiplex Stable Isotope Dimethyl Labeling Coupled with MALDI-MS for Quantitative N-Glycomics**; He Zhu[1]; Cheng Ma[1]; Peng George Wang[1]; [1]Georgia State University, Atlanta, GA

ThP 083 **An Investigation of Ion Adduction for Enhancing Trisaccharide Isomer Separation and Collision Cross Section Identification through TWIMS Analysis**; Jessica Minnick[1]; Eric D. Dodds[1]; [1]University of Nebraska - Lincoln, Lincoln, NE

ThP 084 **Separation and Identification of Sulfated Glycosaminoglycans in Urine using Capillary**

Electrophoresis and Tandem Mass Spectrometry; Patience Sanderson[1]; Xiaorui Han[2]; Fuming Zhang[2]; Robert Linhardt[2]; I. Jonathan Amster[1]; *[1]University of Georgia, Athens, GA; [2]Rensselaer Polytechnic Institute, Troy, NY*

ThP 085 **A Method for the Rapid Determination of Polysaccharide Structures**; Eshani Nandita[1]; Matthew J. Amicucci[1]; Ace G. Galermo[1]; Juan J. Castillo[1]; Carlito B. Lebrilla[1]; *[1]UC Davis, Davis, CA*

DATA-DEPENDENT ACQUISITION
086-092

ThP 086 **Deep Quantitative Phosphoproteomics by Data Independent Acquisition Mass Spectrometry**; Reta Birhanu Kitata[1]; Chia-Feng Tsai[2]; Pei-Yi Lin[1]; Wai-Kok Choong[3]; Yun-Chien Chang[1]; Bo-Shiun Chen[1,4]; Alexey I. Nesvizhskii[5]; Ting-Yi Sung[3]; Yu-Ju Chen[1]; *[1]Institute of Chemistry, Academia Sinica, Taipei City, Taiwan; [2]Pacific Northwest National Laboratory, Richland, WA; [3]Institute of Information Science, Academia Sinica, Taipei City, Taiwan; [4]Department of Chemistry, National Taiwan University, Taipei City, Taiwan; [5]Department of Computational Medicine and Bioinformatics and Department of Pathology, Ann Arbor, Michigan*

ThP 087 **Machine Learning on SpectroMine Results Applied to an Efficient Large-Scale Library Generation Experiment**; Lynn Verbeke[1]; Jan Muntel[1]; Timothy Man[1]; Tejas Gandhi[1]; Aljaz Baumkircher[1]; Oliver M. Bernhardt[1]; Ian Lienert[1]; Roland Bruderer[1]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland*

ThP 088 **Identification of Off-Target Protein-Small Molecule Interactions Using Cellular Thermal Shift Assay (CETSA) and Phase-Constrained Spectrum Deconvolution (ΦSDM) MS Data Acquisition**; Clifford Phaneuf[1]; Antonius Koller[2]; Konstantin Aizikov[3]; Dmitry Grinfeld[3]; Arne Kreutzmann[3]; Daniel Mourad[3]; Oliver Lange[3]; Alexander A Makarov[3]; Lilu Guo[1]; Harvey Lieberman[1]; Aharon Cohen[1]; Alexei Belenky[1]; Alexander R Ivanov[2]; *[1]Sanofi, Waltham, MA; [2]Northeastern University, Boston, MA; [3]Thermo Fisher Scientific, Bremen, Germany*

ThP 089 **Peptide Identification Improvement on a Trapped-Ion-Mobility quadrupole-Time-Of-Flight Mass Spectrometer (TIMS-QTOF) by Optimized Parallel Accumulation Serial Fragmentation (PASEF) Acquisition**; Markus Lubeck[1]; Jens Decker[1]; Andreas Germanus[1]; Michael Krause[1]; Stephanie Kaspar-Schoenefeld[1]; Victor Fursey[2]; Oliver Raether[1]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Bruker Daltonics Inc., Billerica, MA*

ThP 090 **Mapping Protein Interactions Using Data-Dependent Acquisition without Dynamic Exclusion**; Shen Zhang[1]; Brett Larsen[2]; Cassandra Wong[2]; Anne-Claude Gingras[2]; *[1]Lunenfeld-Tanenbaum Research Institute, Sinai Health System, Toronto; [2]Lunenfeld-Tanenbaum Research Institute, Sinai Health System, Toronto, ON*

ThP 091 **Development of Screening Method for Targeted and Undiscovered Per- and polyfluoroalkyl Substances in Surface Water on Q-TOF Mass Spectrometer**; Jun Xiang Lee[1]; Jie Xing[1]; Shiau Hang Tee[2]; Timothy Yan Ann Lim[3]; Zhaoqi Zhan[1]; *[1]Shimadzu Asia Pacific, Singapore, Singapore; [2]School of Physical and Mathematical Sciences, Nanyang Technological University, 21 Nanyang Link SPMS-04-01, Singapore 627371, Singapore, Singapore; [3]National University of Singapore, Singapore, Singapore*

ThP 092 **Mass Fractionation in the Survey Data Improve Protein Identification in Data Dependents Acquisition for Complex Proteome Samples**; Faraz Rashid[1]; Dipankar Malakar[1]; Nirpendra Singh[2]; Manoj Pillai[1]; *[1]SCIEX, Gurgaon, India; [2]Advanced Technology Platform Centre,RCB, Faridabad, India*

DATA-INDEPENDENT ACQUISITION
093-111

ThP 093 **Quantitative Proteomic and Phosphoproteomic Elucidation of Cancer Aneuploidy**; Alison M. Taylor[1]; Wenxue Li[2]; Sejal Jain[1]; Matthew Meyerson[1]; Yansheng Liu[2,3]; *[1]Department of Medical Oncology, Dana-Farber Cancer Institute, Boston, MA; [2]Yale Cancer Biology Institute, West Haven, CT; [3]Department of Pharmacology, Yale University School of Medicine, New Haven, CT*

ThP 094 **Ultra-High Resolution 2D-FTMS for Truly DIA Analysis of Challenging Systems**; Christopher Andrew Wootton[1]; Tomos E. Morgan[1]; Bryan P. Marzullo[1]; Yuko P. Y. Lam[1]; Diana C. Palacio Lozano[1]; Alina Theisen[1]; Anisha Haris[1]; Mark P. Barrow[1]; Peter B. O'Connor[1]; *[1]University of Warwick, Coventry, United Kingdom*

ThP 095 **Low ppm Detection of Host Cell Proteins (HCPs) in Biotherapeutics with Optimised Orbitrap-Based UHPLC HRAM MS**; Amy J Claydon[1]; Tom Buchanan[1]; Philip J. Widdowson[1]; Janusz Debski[1]; Andrew Williamson[2]; Rowan Moore[2]; *[1]Thermo Fisher Scientific, Runcorn, United Kingdom; [2]Thermo Fisher Scientific, Hemel Hempstead, United Kingdom*

ThP 096 **Accelerating DIA Studies to Extend Workflow Utility, Using Ultra-Fast Microflow LC Gradients**; Christie Hunter[1]; Nick Morrice[2]; Zuzana Demianova[3]; *[1]SCIEX, Redwood City, CA; [2]SCIEX, Warrington, United Kingdom; [3]SCIEX, Darmstadt, Germany*

ThP 097 **SWATH-MS for Quantification of Mass Isotopologue Distribution of Cellular Metabolites and Fragments Labeled with Isotopic 13C Carbon in Cyanobacteria**; Damini Jaiswal[1]; Charulata B Prasannan[1,2]; John I Hendry[1]; Pramod P Wangikar[1,2,3]; *[1]Department of Chemical Engineering,Indian Institute of Technology Bombay, Mumbai, India; [2]DBT-Pan IIT Center for Bioenergy, Indian Institute of Technology Bombay, Mumbai, India; [3]Wadhwani Research Center for Bioengineering, Indian Institute of Technology Bombay, Mumbai, India*

ThP 098 **Designing Data Independent Acquisition Methods for Orbitrap Instruments**; Léon Reubsaet[1,2]; Michael Sweredoski[2]; Annie Moradian[2]; Spiros D Garbis[2]; *[1]Department of Pharmaceutical Chemistry, School of Pharmacy, University of Oslo, Oslo, Norway; [2]California Institute of Technology, Pasadena, CA*

ThP 099 **Rapid Proteome Analysis with Data-Independent Acquisition and Super-Rsolution Orbitrap Mass Spectrometry**; Florian Meier[1]; Arne Kreutzmann[2]; Daniel Mourad[2]; Konstantin Aizikov[2]; Dmitry Grinfeld[2]; André C Michaelis[1]; Oliver Lange[2]; Alexander A Makarov[2]; Matthias Mann[1,3]; *[1]Max Planck Institute of Biochemistry, Martinsried, Germany; [2]Thermo Fisher Scientific, Bremen, Germany; [3]NNF Center for Protein Research University of Copenhagen, Copenhagen, Denmark*

ThP 100 **Assessment of Type 2 Diabetes Based upon Quantification of Plasma Proteomes**; Zhilong Lin[1,2]; Guixue Hou[1,2]; Siqi Li[1,2]; Rongli Zhao[1,2]; Huanzi Zhong[1,2]; Fangming Yang[1,2]; Huanming Yang[1,3]; Siqi Liu[1,2]; Yan Ren[1,2]; *[1]BGI-Shenzhen, Shenzhen, China; [2]China National GeneBank, Shenzhen, China; [3]James D. Watson Institute of Genome Sciences, Hangzhou, China*

ThP 101 **Identification and Quantification of Host Cell Proteins in Recombinant Therapeutic Proteins Using Data-Independent Acquisition Mass Spectrometry**; Hongbin Zhu[1]; David Keire[1]; Hongping Ye[1]; *[1]FDA, St. Louis, MO*

ThP 102 **Cysteine-DIA – the Use of Cysteine-Containing Peptides to Increase the Protein Coverage in DIA**; Muhammad Tahir[1]; Arkadiusz Nawrocki[1]; Martin Røssel Larsen[1]; *[1]Department of Biochemistry and Molecular Biology, University of Southern Denmark, Odense, Denmark*

ThP 103 **Effect of Aerobic Exercise on PBMC Protein Profile in Insulin Resistant (IR) and Insulin Sensitive (IS) Participants**; Kevin Paul Erazo Castillo[1]; Sara Ahadi[1]; Kevin Contrepois[1]; Fredrik Edfors[1]; Daniel Hornburg[1]; Si Wu[1]; Francois Haddad[1]; Michael Snyder[1]; [1]*Stanford University, Stanford, CA*

ThP 104 **Characterization of the Insolublome in Aging and Age-related Diseases Using Mass Spectrometry with Data-Independent Acquisitions (DIA/SWATH)**; Xueshu Xie[1]; Manish Chamoli[1]; Dipa Bhaumik[1]; Kathleen Dumas[1]; Renuka Sivapatham[1]; Suzanne Angeli[1]; Anja Holtz[1]; Julie Andersen[1]; Birgit Schilling[1]; Gordon J. Lithgow[1]; [1]*Buck Institute, Novato, CA*

ThP 105 **Elucidation of Organic Micropollutants Biodegradation Using Data-Independent Acquisition as Part of a Drinking Water Filter Process**; Morgan Solliec[1]; Veronika Storck[1]; Benoit Barbeau[1]; [1]*Polytechnique Montréal, Montréal, QC*

ThP 106 **Relative Quantitation of Aqueous Humor Proteins in a Juvenile Rabbit Model of Lensectomy Using Data Dependent and Data Independent Acquisition**; Theodore R. Keppel[1]; Jonathon B. Young[1]; Christine M.B. Skumatz[1]; Alexander E. Salmon[1]; Rebekah L. Gundry[1]; Iris S. Kassem[1]; [1]*Medical College of Wisconsin, Milwaukee, WI*

ThP 107 **Employing Scanning SWATH to Support High Flow Proteomics Sample Acquisition**; Nic Bloomfield[1]; Gordana Ivosev[1]; Fras Wasim[1]; Stephen Tate[1]; Christoph B Messner[2]; Vadim Demichev[2]; Spyros Vernardis[2]; [1]*SCIEX, Concord, ON;* [2]*The Francis Crick Institute, London, United Kingdom*

ThP 108 **HLA-DO / H2-O Modulates the Diversity of the MHC class II Self Peptide Repertoire**; Padma P Nanaware[1]; Mollie M Jurewicz[1]; John D Leszyk[1]; Scott A Shaffer[1]; Lawrence Stern[1]; [1]*University of Massachusetts Medical School, Worcester, MA*

ThP 109 **Targeted Detection of Enzyme Active-site Peptides *via* Data-Independent Selective Infrared Multiphoton Dissociation Liquid Chromatography/Mass Spectrometry**; Nicholas Borotto[1]; Melanie Cheung-Seekit[1]; Chunyi Zhao[2]; Andrew H. Lowell[1]; Jennifer Schmidt[1]; Kinshuk Srivastava[3]; Brandon T. Ruotolo[4]; David H. Sherman[1]; Brent R Martin[4]; Kristina Hakansson[1]; [1]*University of Michigan, Ann Arbor, MI;* [2]*University of Michigan, Ann Arbor, Michigan;* [3]*University of Michigan, Ann Arbor, MI;* [4]*Univeristy of Michigan, Ann Arbor, MI*

ThP 110 **Use of DIA SWATH to Determine the Operational Envelope of a Synthetic Gene Circuit in Vibrio Natriegens**; Mary Ashley Rimmer[1]; W Judson Hervey, IV[2]; Dagmar H Leary[2]; Robert G Egbert[3]; Enoch Yeung[4]; Gary J Vora[2]; [1]*NRC Post-doctoral Fellow, US Naval Research Laboratory, Washington, D.C.;* [2]*Center for Bio/Molecular Science & Engineering, US Naval Research Laboratory, Washington, D.C.;* [3]*Pacific Northwest National Laboratory, Richland, WA;* [4]*University of Santa Barbara, Santa Barbara, CA*

ThP 111 **Fiber Supplements Induce Protein Variation on a Diverse Cohort: A Pilot Study**; Jeniffer Quijada[1]; Samuel M. Lancaster[1]; Brittany Ann Lee[1]; Daniel Hornburg[1]; Sara Ahadi[1]; Si Wu[1]; Michael Snyder[1]; [1]*Stanford University School of Medicine, Stanford, CA, 94305*

DISEASE BIOMARKERS II
112-130

ThP 112 **Capillary Electrophoresis-Mass Spectrometry-Based Identification of Unique Metabolic Profiles in Neurodegenerative Clinical Samples**; Kaylie I Kirkwood[1]; Tharani Sabaretnam[2]; Gilles J Guillemin[2]; David C Muddiman[1]; [1]*North Carolina State University, Raleigh, NC;* [2]*Macquarie University, Sydney, NSW, Australia*

ThP 113 **Identification of Candidate Biomarkers for Early Prediction of Prostate Cancer Progression Using Targeted Proteomics on Organ-confined Primary Tumors**; Yuqian Gao[1]; Yi-Ting Wang[1]; Hui Wang[1]; Denise Young[2]; Yongmei Chen[2]; Yingjie Song[2]; Athena A. Schepmoes[1]; Thomas L. Fillmore[1]; Tujin Shi[1]; Wei-Jun Qian[1]; Richard D. Smith[1]; Sudhir Srivastava[3]; Jacob Kagan[3]; Albert Dobi[2]; Inger L. Rosner[2]; Isabell A. Sesterhenn[4]; Shiv Srivastava[2]; Gyorgy Petrovics[2]; Karin D. Rodland[1]; Jennifer Cullen[2]; Tao Liu[1]; [1]*Pacific Northwest National Laboratory, Richland, WA;* [2]*Walter Reed National Military Medical Center, Bethesda, MD;* [3]*National Cancer Institute, Bethesda, MD;* [4]*Joint Pathology Center, Silver Spring, MD*

ThP 114 **Early Detection Hepatocellular carcinoma *via* MRM-MS with a Serum Protein-based Multi-marker panel: A Large-Scale Multicenter study**; Injoon Yeo[1]; Hyunsoo Kim[2, 3, 4]; Ji Hyeon Lee[5]; Young-Suk Lim[6, 7]; Youngsoo Kim[2, 5, 8]; [1]*Departments of Biomedical Engineering, Seoul National University College of Medicine, Seoul, South Korea;* [2]*Departments of Biomedical Engineering, Seoul National University College of Medicine, Jongro-gu, South Korea;* [3]*Department of Biomedical Sciences, Seoul National University College of Medicine, Seoul, South Korea;* [4]*Institute of Medical and Biological Engineering, Medical Research Center, Seoul National University College of Medicine, Seoul, South Korea;* [5]*Department of Biomedical Sciences, Seoul National University College of Medicine, Jongro-gu, South Korea;* [6]*Department of Gastroenterology, University of Ulsan College of Medicine, Seoul, South Korea;* [7]*Liver center, Asan Medical Center, Seoul, South Korea;* [8]*Institute of Medical and Biological Engineering, Medical Research Center, Seoul National University College of Medicine, Jongro-gu, South Korea*

ThP 115 **LESA Sampling of Human Non-Alcoholic Fatty Liver Disease Tissue for the Profiling of Liver Fatty Acid Binding Protein**; James W Hughes[1]; Iain B Styles[1]; Patricia F Lalor[1]; Helen J Cooper[1]; [1]*University of Birmingham, Birmingham, United Kingdom*

ThP 116 **Top-Down Mass Spectrometry of Appendix Derived Synuclein Proteoforms and Their Role in Parkinson Disease**; Bryan A Killinger[1]; Zachary Madaj[1]; Jacek W Sikora[2]; Nolwen Rey[1, 3]; Alec J Haas[1]; Yamini Vepa[1]; Daniel Lindqvist[4, 5]; Honglei Chen[6]; Paul M Thomas[2]; Patrik Brudin[1]; Lena Brudin; Neil L Kelleher[2]; Viviane Labrie[1, 7]; [1]*Center for Neurodegenerative Science, Van Andel Research Institute, Grand Rapids, Michigan;* [2]*Proteomics Center of Excellence, Northwestern University, Chicago, ILLINOIS;* [3]*Paris-Saclay Institute of Neuroscience, Centre National de la Recherche Scientifique, Gif-sur-Yvette, France;* [4]*Department of Clinical Sciences, Psychiatry, Faculty of Medicine, Lund University, Lund, Sweden;* [5]*Psychiatric Clinic, Lund, Division of Psychiatry, Lund, Sweden;* [6]*Department of Epidemiology and Biostatistics, College of Human Medicine, Michigan State University, East Lansing, Michigan;* [7]*Centre for Addiction and Mental Health, Toronto, Ontario*

ThP 117 **Identifying Neoantigens for Personalized Cancer Vaccines by Personalized *de novo* Peptide Sequencing**; Rui Qiao[1]; Ngoc Hieu Tran[1]; Lei Xin[2]; Xin Chen[2]; Baozhen Shan[2]; Ming Li[1]; [1]*University of Waterloo, Waterloo, ON;* [2]*Bioinformatics Solutions Inc., Waterloo, ON*

ThP 118 **Novel Method for Screening of ADA-SCID in DBS, in Addition to 2nd Tier Methodology**; Jessica B Hendricks; *Centers for Disease Control and Prevention, Atlanta, GA*

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of Neurology, Emory University, Atlanta, GA; [3]Department of Psychiatry and Behavioral Sciences, Emory University, Atlanta, Georgia; [4]Department of Human Genetics, Emory University, Atlanta, GA

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ThP 139 **Limited Proteolysis Coupled to Mass Spectrometry, a Novel Drug Target Deconvolution Strategy**; Nigel Beaton[1]; Roland Bruderer[1]; Ilaria Piazza[2]; Paola Picotti[2]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland; [2]ETH Zurich, Zurich, Switzerland*

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ThP 186 **Qualitative and Quantitative Analysis of Pork in Beef Food by LC-MS/MS**; Qiaoxia Liu[1]; Qiang Li[2]; Hongyuan Hao[2]; Taohong Huang[2]; *[1]Shimadzu (China) Co., LTD. Shanghai Branch, Shanghai, China; [2]Shimadzu (China) Co., LTD. Shanghai Branch, Shanghai, China*

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ThP 190 **Charge Transfer Dissociation of Vitamin B12**; Halle M Edwards[1]; Zachary J. Sasiene[1]; Praneeth M Mendis[1]; Glen P Jackson[1,2]; *[1]C. Eugene Bennett Department of Chemistry, West Virginia University, Morgantown, WV; [2]Department of Forensic and Investigative Science, West Virginia University, Morgantown, WV*

ThP 191 **LC-MS/MS Method for Sensitive Detection and Quantitation of 8 Water-Soluble vitamins in Infant Milk Powder**; Yin Ling Chew[1]; Eleanor Wai Yi Hor[2]; Qi Zong Lee[3]; Noah Luzheng Ong[3]; Muhammad Averus[4]; Suwiton Suwiton[4]; Martin Uli Tua[4]; Jie Xing[1]; Zhaoqi Zhan[1]; *[1]Shimadzu (Asia Pacific) Pte Ltd, Singapore, Singapore; [2]School of Physical and Mathematical Sciences, Nanyang Technological University, 21 Nanyang Link SPMS-04-01, Singapore 627371, Singapore, Singapore; [3]National University of Singapore, Singapore, Singapore; [4]PT Saraswanti Indo Genotech, Bogor, Indonesia*

ThP 192 **GC-MS Combined with Chemometrics Reveals the Difference in Volatile Metabolic Profile Between High Yield and Normal Yield Royal Jelly**; Dandan Qi[1]; Chengying Ma[2]; Wenwen Wang[3]; Jianke Li[1]; *[1]Institute of Apicultural Research / Key Laboratory of Pollinating Insect Biology, Ministry of Agriculture, Chinese Academy of Agricultural Sciences, Beijing, China; [2]Tea Research Institute, Guangdong Academy of Agricultural Sciences, Guangzhou, China; [3]Agilent Technologies Co. Ltd, Beijing, China*

ThP 193 **Simultaneous Measurement of Key Odorants at their Sensory Thresholds in Juice Grapes**; Terry L Bates[1]; Madeline Y Bee[2]; Xuéfei Kuang[2]; Gavin L. Sacks[2]; *[1]Cornell, Ithaca, NY; [2]Cornell University, Ithaca, NY*

ThP 194 **High-Resolution Mass Spectrometry Informs the Selection of Food Processing Parameters for the Large-Scale Enzymatic Release of N-glycans from Milk Glycoproteins**; Apichaya Bunyatratchata[1]; Yu-Ping Huang[1]; Gulustan Ozturk[1]; Juliana Maria Leite Nobrega De Moura Bell[1]; Daniela Barile[1,2]; *[1]Department of Food Science and Technology, University of California, Davis, California; [2]Foods for Health Institute, University of California, Davis, California*

ThP 195 **A Novel Sensitive LC-MSMS Method for Porcine Gelatin Detection in Cosmetic and Confectionary Products**; Nurul Atiqah Sa'don[1]; Charles T. Yang[2]; Dipankar Ghosh[2]; Tristan chia[3]; Fiona Teh Hui Boon[4]; Chris Cheah[4]; *[1]Halvec Laboratories Sdn. Bhd, Selangor Darul Ehsan, Malaysia; [2]Thermo Fisher Scientific, San Jose, CA; [3]Thermo Fisher Scientific, Selangor, Malaysia; [4]Thermo Fisher Scientific, Singapore, Singapore*

ThP 196 **Rapid Evaporative Ionisation Mass Spectrometry for Detecting Compounds Related to Consumer Liking of Grilled Lamb**; Alastair Ross[1]; Paul Middlewood[1]; Stefan Clerens[1]; Patricia L Johnson[2]; Patrick Silcock[3]; Graham T Eyres[3]; Carolina E Realini[4]; *[1]AgResearch Ltd, Lincoln, New Zealand; [2]AgResearch Ltd, Invermay, New Zealand; [3]University of Otago, Dunedin, New Zealand; [4]AgResearch Ltd, Palmerston North, New Zealand*

ThP 197 **Detecting Insult-Induced Protein-Protein Crosslinks Formed During Food Processing**; Hannah McKerchar[1,2,3,4]; Jolon M Dyer[2,3,4]; Evelyne Maes[3]; Juliet A. Gerrard[2,4,5]; Renwick C. J Dobson[1,2,4]; Stefan Clerens[2,6,7]; *[1]University of Canterbury, Christchurch, New Zealand; [2]Biomolecular Interaction Centre, Christchurch, New Zealand; [3]AgResearch Ltd, Lincoln, New Zealand; [4]Riddet Institute, Massey University, Christchurch, New Zealand; [5]University of Auckland, Auckland, New Zealand; [6]AgResearch Ltd, Lincoln, New Zealand; [7]Riddet Institute, Massey University, Palmerston North, New Zealand*

ThP 198 **Untargeted Metabolomics: A Path Towards Objective Measures of Dietary Intake in Human Studies**; Julia M Gauglitz[1]; Ricardo da Silva[1]; Alan K Jarmusch[1]; Francesca Di Ottavio[1,2]; Morgan Panitchpakdi[1]; Elizabeth A Brown[1]; Christine M Aceves[1]; Ming Wang[1]; Bohan Ni[1]; Nicole Sikora[1]; Rachel J Dutton[3]; Rob Knight[4]; Pieter Dorrestein[1]; *[1]Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego, La Jolla, CA; [2]Faculty of Bioscience and Technology for Food, Agriculture and Environment, University of Teramo, Teramo, Italy; [3]Division of Biological Sciences, University of California San Diego, La Jolla, CA; [4]Department of Pediatrics, University of California San Diego, La Jolla, CA*

ThP 199 **Combining Sensory and Chemical Analyses (GC-MS) to Evaluate Shelf Stability Related to Storage Condition for an American IPA Beer**; Joseph E Binkley[1]; Elizabeth Humston-Fulmer[2]; Lorne Fell[2]; *[1]LECO Corporation, St. Joseph, MI; [2]LECO Corporation, St Joseph, MI*

ThP 200 **Droplet-based Desorption of Trace Volatiles Following Parallel Headspace Extraction onto Sorbent Sheets**; Madeleine Y Bee[1]; Jessica P Rafson[1]; Gavin L. Sacks[1]; *[1]Cornell University, Ithaca, NY*

ThP 201 **Comprehensive Characterization of Eight Different Olive Tree Derived Matrices Using LC-ESI/APCI-QTOF and GC-APCI-QTOF and a Non-Targeted Software Workflow**; Lucía Olmo-García[1]; Karin Wendt[2]; Alberto Fernández-

Gutiérrez[1]; Nikolas Kessler[2]; Heiko Neuweger[2]; Cory Lytle[3]; José María Olmo-Peinado[4]; Carsten Baessmann[2]; Alegría Carrasco-Pancorbo[1]; *[1]Department of Analytical Chemistry, Faculty of Science, University of Granada, Granada, Spain; [2]Bruker Daltonik GmbH, Bremen, Germany; [3]Bruker Daltonics Inc., Billerica, MA; [4]Acer Campestres S.L. Almendro, Jaén, Spain*

ThP 202 **Discovery and Targeted Peptidomics Revealed pH-Dependent Enzyme-Substrate Interactions of Endogenous Proteolysis in Human Milk**; Junai Gan[1]; Jingyuan Zheng[1]; Nithya Krishnakumar[1]; Elisha Goonatilleke[1]; Carlito B. Lebrilla[1]; Daniela Barile[1]; J. Bruce German[1]; *[1]University of California, Davis, CA*

ThP 203 **Analyses of Water-Soluble and Fat-Soluble Vitamins in Fruits Juice by Triple Quadrupole LC/MS**; Seiya Tanaka[1]; Masako Yorishita[2]; *[1]Agilent Technologies, Hachioji City, Japan; [2]ITOEN, LTD, Shibu-ya-ku, Japan*

GLYCOPROTEINS II
204-224

ThP 204 **Measuring Statistical Similarity of Glycosylation between Influenza A Virus Variants**; Deborah K Chang[1]; William E Hackett[2]; Joshua A Klein[2]; Joseph Zaia[1,2]; *[1]Boston University School of Medicine, Boston, MA; [2]Boston University, Boston, MA*

ThP 205 **A Facilely Synthesized Glutathione-Functionalized Silver Nanoparticles-Grafted Covalent Organic Framework for Rapid and Highly Efficient Enrichment of N-Linked Glycopeptides**; Yu-Fang Ma[1]; Li-Juan Wang[1,2]; Ying-Lin Zhou[1]; Xin-Xiang Zhang[1]; *[1]Peking University, Beijing, China; [2]Hebei University, Baoding, China*

ThP 206 **Enzymatic Tagging of Glycoproteins on the Cell Surface for Their Global and Site-Specific Analysis with Mass Spectrometry**; Fangxu Sun[1]; Suttipong Suttapitugsakul[1]; Ronghu Wu[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

ThP 207 **An Effective Chemical Method to Catch Low-Abundance Glycoproteins for MS Analysis**; Ronghu Wu[1]; Haopeng Xiao[1]; Suttipong Suttapitugsakul[1]; Fangxu Sun[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

ThP 208 **Improved Profiling of Sialylated N-Linked Glycans by Ion Chromatography-Orbitrap Mass Spectrometry**; Sachin Patil[1]; Jeffrey Rohrer[1]; *[1]Thermo Fisher Scientific, Sunnyvale, CA*

ThP 209 **Rapid Characterization of Domain-Specific [Fc vs. Fab] Glycosylation in Monoclonal Antibodies (mAbs)**; Charles Nwosu[1]; Mei Zhu[2]; Lei Wang[1]; Anne Kowal[1]; *[1]Takeda Pharmaceuticals International Co, Cambridge, MA; [2]Takeda Pharmaceuticals, International Co., Cambridge, MA*

ThP 210 **Glycoproteomic Analysis of Cells Containing Unnatural Monosaccharides**; Yixuan (Axe) Xie[1]; Ying Sheng[1]; Qiongyu Li[1]; Maurice Wong[1]; Qingwen (Dave) Zhou[1]; Carlito B. Lebrilla[1]; *[1]University of California, Davis, CA*

ThP 211 **Simultaneously Identifying and Distinguishing Glycoproteins with O-GlcNAc and the Tn Antigen in Human Cancer Cells**; Senhan Xu[1]; Jiangnan Zheng[1]; Haopeng Xiao[2]; Ronghu Wu[1]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]Harvard Medical School, boston, MA*

ThP 212 **Chemical Derivatization for Fine Mapping of Glycopeptides in EThcD MS**; Ying Zhang[1]; Lijun Yang[2]; Haojie Lu[2]; *[1]Fudan University, Shanghai, China; [2]Fudan University, Shanghai, China*

ThP 213 **Confident and Efficient Characterization of Recombinant Human Follicle Stimulating Hormone with the Thermo Scientific Q Exactive HF-X BioPharma Platform**; Xiaoxi Zhang[1]; Philip J. Widdowson[2]; Rowan Moore[2]; *[1]ThermoFisher Scientific, Shanghai, China; [2]Thermo Fisher Scientific, Hemel Hempstead, UK, Hemel Hempstead, United Kingdom*

ThP 214 **MS-Based Workflow for the Characterization of Glyco-Engineered Therapeutic Glycoproteins with Oligo/Poly-Sialic Acids in Bacteria**; Chia-wei Lin[1]; Hanne L.P. Tytgat[2]; Timothy G. Keys[2]; Markus Aebi[2]; *[1]Functional Genomic Center Zürich, Zurich, Switzerland; [2]Institute of Microbiology, ETHZ, Zurich, Switzerland*

ThP 215 **Identification of N-Glycopeptides with MetaMorpheus**; Lei Lu[1]; Michael R Shortreed[1]; Robert J Millikin[1]; Mark Scalf[1]; Lloyd M Smith[1]; *[1]University of Wisconsin-Madison, Madison, WI*

ThP 216 **N-Glycan Sub-Type as a Pathogenic Factor in Influenza**; Lisa Parsons[1]; John F. Cipollo[1]; Yanming An[1]; Li Qi[2]; Jeffery K. Taubenberger[2]; Kevan Hartshon[3]; Mitchell White[3]; *[1]FDA, Silver Spring, MD; [2]NIH/NIAID, Bethesda, MD; [3]Boston University School of Medicine, Boston, MA*

ThP 217 **Construction of a Structure and Site Specific Glycopeptide Transition Library for Glycopeptide Quantitation by DIA/SWATH**; Miloslav Sanda[1]; Nathan J Edwards[2]; Julius Benicky[1]; Zuzana Brnakova Kenedy[1]; Radoslav Goldman[1,2]; *[1]Georgetown University, Lombardi Cancer Center, Washington, DC; [2]Georgetown University, Department of Biochemistry and Molecular & Cellular Biology, Washington, DC*

ThP 218 **High-Throughput and Site-Specific N-Glycosylation Analysis of Human Alpha-1-Acid Glycoprotein**; Toma Keser[1]; Gordan Lauc[1,2]; Mislav Novokmet[2]; *[1]Faculty of pharmacy and biochemistry, University of Zagreb, Zagreb, Croatia; [2]Genos, Glycoscience Laboratory, Borongajska cesta 83h, Zagreb, Croatia*

ThP 219 **Mass Spectrometric Elucidation of Global Glycosylation Profile on a Fungal Vaccine Adjuvant BL-ENG2**; Junfeng Huang[1]; Lucas dos Santos Dias[2]; Marcel Wüthrich[2]; Lingjun Li[1,3]; *[1]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [2]Department of Pediatrics, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI; [3]Department of Chemistry, University of Wisconsin-Madison, Madison, WI*

ThP 220 **Effects of In-Source Supercharging and Subcharging for Glycopeptide Analysis in a Trapped Ion Mobility Quadrupole Time-of-Flight Mass Spectrometer**; Kristina Marx[1]; Hans J.C.T. Wessels[2]; Pierre-Olivier Schmit[3]; Alain J. Van Gool[2]; Dirk J. Lefeber[2]; *[1]Bruker Daltonik GmbH, Bremen, Germany; [2]Translational Metabolic Laboratory, Department of Laboratory medicine, Radboudumc, Nijmegen, Netherlands; [3]Bruker Daltonique S.A, Wissembourg, France*

ThP 221 **Analysis of N- and O-Glycosylation on a Highly Glycosylated Protein Highlights Potential Sources of Error When Sequencing Intact Glycopeptide Spectra**; Gary Wilson[1]; Miyoshi Haruta[2,3]; Alexander Hebert[1]; Michael S Westphall[1]; Michael Sussman[2,3]; Joshua Coon[1,3,4,5]; *[1]Department of Chemistry, University of Wisconsin, Madison, WI; [2]Department of Biochemistry, University of Wisconsin,, Madison, WI; [3]Genome Center of Wisconsin, Madison, WI; [4]Morgridge Institute for Research, Madison, WI; [5]Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI*

ThP 222 **GlyProSILC: Glycan/Protein Stable Isotope Labeling in Cell Cultures Approach for Concurrent Glycomics/Proteomics/Glycoptoeomics Analysis**; Wenjing Peng[1]; Jingfu Zhao[2]; Mona Goli[2]; Yehia Mechref[2]; *[1]Texas Tech University, Lubbock, TX; [2]Department of Chemistry and Biochemistry, Texas Tech University, Lubbock, Texas*

ThP 223 **LC-MS/MS Characterization of Isomeric Glycopeptides Using Extra-long C18 Column**; Aiying Yu[1]; Yifan Huang[1]; Jingfu Zhao[1]; Xue Dong[1]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX*

ThP 224 **Elucidating the Glycan Structures of the Archaea *Methanosarcina acetivorans* and *Methanosarcina barkeri* by Mass Spectrometry**; Deborah R Leon[1]; Cheng

Lin[1]; Rachel R. Ogorzalek Loo[2]; Joseph A Loo[2]; Robert P. Gunsalus[2]; Catherine E. Costello[1]; *[1]Boston University School of Medicine, Boston, MA; [2]University of California LA, Los Angeles, CA*

IMAGING MS: DISEASE MARKERS II
225-242

ThP 225 **Bifunctional Cleavable Probe for *in-situ* Multiplexed Glycan Detection and Imaging Using Mass Spectrometry**; Wen Ma[1]; Shuting Xu[1]; Yu Bai[1]; Huwei Liu[1]; *[1]Peking University, Beijing, China*

ThP 226 **DESI-IMS Revealed the Association of Linoleic Acid, Oleic Acid and Arachidonic Acid in the Rupture of Cerebral Aneurysm**; Ariful Islam[1]; Ririko Takeda[2]; Tomohito Sato[1]; Hiroki Kurita[3]; A s m Waliullah[1]; Md. Al Mamun[1]; Makoto Horikawa[1,4]; Mitsutoshi Setou[1,4]; *[1]Department of Cellular and Molecular Anatomy, Hamamatsu University School of Medicine, Hamamatsu, Japan; [2]Department of Neurosurgery, Mizonokuchi Hospital, Teikyo University School of Medicine, Kanagawa, Japan, Kawasaki, Japan; [3]Department of Cerebrovascular Surgery, Saitama Medical University International Medical Center, Hidaka, Saitama, Japan, Hidaka, Japan; [4]International Mass Imaging Center, Hamamatsu University School of Medicine,, Hamamatsu, Japan*

ThP 227 **Multimodal MALDI IMS to Visualize Staphylococcal Molecular Adaptation within the Infectious Microenvironment**; William J Perry[1,2,3]; Jeffrey M. Spraggins[1,2,4]; Caroline M. Grunenwald[3,5]; Jessica R Sheldon[3,5]; Eric P. Skaar[3,5]; Richard M. Caprioli[1,2,4,6,7]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Department of Chemistry, Vanderbilt University, Nashville, TN; [3]Vanderbilt Institute for Infection, Immunology, and Inflammation, Vanderbilt University Medical Center, Nashville, TN; [4]Department of Biochemistry, Vanderbilt University, Nashville, TN; [5]Department of Pathology, Microbiology and Immunology, Vanderbilt University School of Medicine, Nashville, TN; [6]Department of Pharmacology, Vanderbilt University, Nashville, TN; [7]Department of Medicine, Vanderbilt University, Nashville, TN*

ThP 228 **MALDI Imaging to Characterise the Lipid Signature of Clinical Prostate Tumours**; Shadrack M Mutuku[1,2]; Paul J Trim[3]; Xander Spotbeen[2,4]; Johan O R Gustafsson[5]; Jessica M Logan[5]; Alexandra Sorvina[5]; Margaret M Centenera[1,2]; Johannes V Swinnen[4]; Marten F Snel[3]; Lisa M Butler[1,2]; *[1]Adelaide Medical School, The University of Adelaide, Adelaide, Australia; [2]Prostate Cancer Research Group, South Australian Health and Medical Research Institute (SAHMRI), Adelaide, Australia; [3]Mass Spectrometry Core Facility, South Australian Health and Medical Research Institute (SAHMRI), Adelaide, Australia; [4]Laboratory of Lipid Metabolism and Cancer, Department of Oncology, LKI-Leuven Cancer Institute, KU Leuven – University of Leuven, Leuven, Belgium; [5]ARC CoE in Convergent Bio-Nano Science & Technology, Future Industries Institute, University of South Australia, Adelaide, Australia; [6]Mechanisms in Cell Biology and Disease Research Group, Cancer Research Institute, University of South Australia, Adelaide, Australia*

ThP 229 **Classification and Identification of Lipid Biomarkers for the Prediction of Melanoma**; Jone Garate[1]; Roberto Fernandez[2]; Lucia Martin-Saiz[2]; Arantza Perez-Valle[2]; Sergio Lage[2]; Veronica Velasco[3]; Aintzane Asumendi[2,3]; Jesus Gardeazabal[3]; Juan Luis Artola[3]; Ignacio Zabalza[4]; Rosa Marti-Laborda[5]; Begoña Ochoa[2]; Maria Dolores Boyano[2,3]; Jose Andres Fernandez[2]; *[1]University of Basque Country, Leioa, Spain; [2]University of Basque Country, Leioa, Spain; [3]Cruces University Hospital, Leioa, Spain; [4]Galdakao-Usansolo Hospital, Galdakao, Spain; [5]Hospital Universitari Arnau de Vilanova, Lleida, Spain*

ThP 230 **Mass Spectrometry Imaging Identifies Altered Lipid Metabolites in the Mouse Testis in Mice Lacking Liver-X Receptors**; Sheba Jarvis[1]; Mark Towers[2]; Charlotte Bevan[1]; Emmanuelle Claude[2]; *[1]Imperial College London, Hammersmith Hospital, London, United Kingdom; [2]Waters Corporation, Wilmslow, United Kingdom*

ThP 231 **Tissue Mass Spectrometry Imaging: Profiling of Secondary Human Lymphoid Organs**; Constantinos Petrovas[1]; Cristina Silvescu[2]; Shannon Cornett[2]; Giulia Fabozzi[1]; Frank Arnold[3]; Paula Lei[3]; *[1]Tissue Analysis Core, VRC, NIAID, NIH, Bethesda, MD; [2]Bruker Daltonics Inc., Billerica, MA; [3]Vaccine Production Program, VRC, NIAID, NIH, Gaithersburg, MD*

ThP 232 **Identification of Therapeutic Targets of Multiple Sclerosis through MALDI - Imaging Mass Spectrometry of Experimental Autoimmune Encephalomyelitis (EAE) Mouse Model**; Nami Tanaka[1]; Hiroki Yamashita[1]; Takashi Nirasawa[2]; Ryo Kajita[2]; Katsutoshi Taguchi[3]; Masaki Tanaka[3]; Takayuki Kondo[4]; Yudai Tsuji[1]; Nobuto Kakuda[1]; Masaya Ikegawa[1]; *[1]Doshisha University, Kyoto, Japan; [2]Bruker Japan K.K., Yokohama, Japan; [3]Department of Anatomy and Neurobiology, Graduate School of Medical Science, Kyoto Prefectural University of Medicine, Kyoto-city, Japan; [4]Kansai Medical University Medical Center, Hirakata, Japan*

ThP 233 **Nanomanipulation-Coupled MALDI Imaging Mass Spectrometry for Single Organelle Analysis to Measure Metabolic Changes responding to Oxidative Stress in Neuroblastoma Cells**; Imesha W. De Silva[1]; R. Scott Duncan[2]; Peter Koulen[2]; Guido F. Verbeck[1]; *[1]University of North Texas, Denton, TX; [2]Vision Research Center, Department of Ophthalmology, School of Medicine, University of Missouri-Kansas City, Kansas City, MO*

ThP 234 **Analysis of Liver Transplant Biopsies for Biomarkers of Transplant Rejection**; Michelle Reyzer[1]; Audra M. Judd[1]; Jennifer L. Harvey[1]; Bryna E. Burell[2]; Drew Lesniak[2]; Anthony Demetrius[2]; Richard M. Caprioli[1]; *[1]Vanderbilt University, Nashville, TN; [2]Immune Tolerance Network, Seattle, WA*

ThP 235 **Characterizing Malignancy Potential of Pancreatic Intraductal Papillary Mucinous Neoplasm (IPMN) Cyst Tissue and Fluid Using Desorption Electrospray Ionization Mass Spectrometry**; Alena Bensussan[1]; John Lin[1]; Sadhna Dhingra[2]; Hop S Tran Cao[3]; Livia S. Eberlin[1]; *[1]The University of Texas at Austin, Austin, TX; [2]Baylor College of Medicine, Houston, TX; [3]MD Anderson Cancer Center, Houston, TX*

ThP 236 **MALDI-MSI Approaches for Visualizing Lipid Markers of Alzheimer's Disease**; Matthias Holzlechner[1]; Daniela D'Amico[1]; Maribel Donoso Rivera[1]; Eliseo Eugenin[1]; Brendan Prideaux[1]; *[1]University of Texas Medical Branch, Galveston, TX*

ThP 237 **Identification of Novel Aldosterone Derivatives on Adrenal Sections of Primary Aldosteronism Patients**; Yuki Sugiura; *Keio University, Tokyo, Japan*

ThP 238 **Dissecting Pathogenesis of Dilated Cardiomyopathy (DCM) on J2N-k Hamster Model Using MALDI-Imaging Mass Spectrometry in Combination with Shotgun Proteomics**; Inori Shintani[1]; Takashi Tsuji[2]; Mizuki Ishida[3]; Takashi Nirasawa[4]; Ryo Kajita[4]; Hatsue Ishibashi-Ueda[5]; Hidetoshi Masumoto[2]; Kenji Minatoya[2]; Masaya Ikegawa[3]; *[1]Doshisha university, Kyotanabe City, Japan; [2]Kyoto University, Kyoto, Japan; [3]Doshisha University, Kyotanabe city, Kyoto, Japan; [4]Bruker Japan K. K., Yokohama, Japan; [5]National Cerebral and Cardiovascular Center Research Institute, Suita, Japan*

ThP 239 **Comprehensive Quantitative Lipidomic Analysis of Mouse Hearts Using AP-SMALDI Mass Spectrometry Imaging and LC-MS/MS**; Vannuruswamy Garikapati[1,2]; Claudia Colasante[2]; Eveline Baumgart-Vogt[2]; Bernhard

Spengler[1]; [1]*Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, Giessen, Germany;* [2]*Institute for Anatomy and Cell Biology II, Division of Medical Cell Biology, Justus Liebig University Giessen, Giessen, Germany*

ThP 240 **3D-Surface AP-SMALDI MS Imaging Reveals Tegument-Specific Lipid Compositions in Human Pathogen *Schistosoma mansoni***; Patrik Kadesch[1]; Thomas Quack[2]; Stefanie Gerbig[1]; Christoph G. Grevelding[2]; Bernhard Spengler[1]; [1]*Institute of Inorganic and Analytical Chemistry, Justus Liebig University Giessen, Giessen, Germany;* [2]*Institute of Parasitology, Giessen, Germany*

ThP 241 **Analysis of Malaria-causing Plasmodia Infected Hepatocytes in Mouse Liver *via* Spatially Targeted Imaging Mass Spectrometry**; Michael D. Tuck[1]; Michelle L. Reyzer[1]; Nathan Heath Patterson[1]; David M. Anderson[1]; Elizabeth Glennon[2]; Adam Lewis[2]; Alexis Kaushansky[2]; Richard M. Caprioli[1]; [1]*Vanderbilt Mass Spectrometry Research Center and Department of Biochemistry, Nashville, TN;* [2]*Center for Infectious Disease Research, Seattle, Washington*

ThP 242 **Multi-Modal Imaging Visualizes HIV-Mediated Cardiac Damage**; Matthias Holzlechner[1]; Eliseo Eugenin[1]; Brendan Prideaux[1]; [1]*The University of Texas Medical Branch (UTMB), Galveston, TX*

IMAGING MS: METHOD DEVELOPMENT II
243-263

ThP 243 **Laser Microdissection-LC-MS/MS Method for Quantitative Tissue Distribution Analysis (QTDA) of Tumor Tissue**; William C. Putnam[1,2]; Raja Reddy Kallem[1,2]; Indhumathy Subramaniyan[1,2]; [1]*Texas Tech University Health Sciences Center - School of Pharmacy, Dallas, TX;* [2]*Clinical Pharmacology and Experimental Therapeutics Center, TTUHSC, Dallas, TX*

ThP 244 **Non-destructive Tissue Lipids Profiling and Imaging Using Tip-Contact Sampling/Ionization Mass Spectrometry**; Xiaoming Chen[1]; Jianmin Wu[1]; [1]*Zhejiang University, Hangzhou, China*

ThP 245 **Combining MALDI Imaging and Liquid Extraction Surface Analysis for Spatial Metabolomics**; Jeremy Wolff[1]; Alain Creissen[2]; Matt Orcutt[2]; Jan H. Kobarg[3]; Shannon Cornett[1]; [1]*Bruker Daltonics Inc., Billerica, MA;* [2]*HTX Technologies, Chapel Hill, NC;* [3]*Bruker Daltonik GmbH, Bremen, Germany*

ThP 246 **Impact of the DIUTHAME for Distribution Analysis of Metabolites on Biological Tissues by DESI-MSI**; Daisuke Saigusa[1]; Masahiro Kotani[2]; Takayuki Ohmura[2]; [1]*Tohoku University, Sendai, Japan;* [2]*Hamamatsu Photonics, Iwata, Japan*

ThP 247 **Automated Mass Spectrometry Imaging of over 2,000 Proteins from Tissue Sections at 100-µm Spatial Resolution**; Paul D. Piehowski[1]; Ying Zhu[1]; Lisa M. Bramer[1]; Kelly G. Stratton[1]; Rui Zhao[1]; Daniel J. Orton[1]; Ronald J. Moore[1]; Jia Yuan[2]; Hugh D. Mitchell[1]; Yuqian Gao[1]; Bobbie-jo M. Webb-robertson[1]; Sudhansu K. Dey[2]; Ryan T. Kelly[1,3]; Richard D. Smith[1]; Kristin E Burnum-Johnson[1]; [1]*Pacific Northwest National Laboratory, Richland, WA;* [2]*Cincinnati Children's Hospital, Cincinnati, OH;* [3]*Brigham Young University, Provo, UT*

ThP 248 **Dual Polarity IMS of Phospholipids from Whole-body Drosophila Tissue Sections**; Ethan Yang[1]; Chiara Gamberi[2]; Pierre Chaurand[1]; [1]*University of Montreal, Montreal, QC;* [2]*Concordia University, Montreal, Qc*

ThP 249 **Lipid Biomarker Candidates for Focal Cerebral Ischemia developed by Dual Polarity Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry Imaging**; Sohee Yoon; *Korea Research Institute of Standards and Science, Daejeon, South Korea*

ThP 250 **MALDI Mass Spectrometry Imaging Reveals Distinct Spatio-Molecular Lipid Distributions in Mouse Lungs**; Caitlin M. Tressler[1]; Cristina Silvescu[2]; Shannon Cornett[2]; Kanchan Sonkar[1]; Ruoqing Cai[1]; Vinay Ayyappan[1]; Oluwatobi Adelaja[1]; Kristine Glunde[1]; [1]*Johns Hopkins University School of Medicine, Baltimore, MD;* [2]*Bruker Daltonics Inc., Billerica, MA*

ThP 251 **Desorption Electrospray Ionization (DESI) and Dielectric Barrier Discharge (DBD) Ionization Mass Spectrometry Imaging of Lipid Metabolism in Alzheimer's Disease**; Isabella James[1]; John C Price[1]; Paul B Farnsworth[1]; Mercede N Erickson[1]; [1]*Brigham Young University, Provo, UT*

ThP 252 **MALDI Imaging of Eucalyptus Leaves from Rust Resistant and Susceptible Genotypes**; Thais Regiani Cataldi[1]; Ilara Gabriela Frasson Budzinski[2]; Andressa Peres Bini[2]; Mônica Teresa Veneziano Labate[2]; Carlos Alberto Labate[2]; [1]*ESALQ, Piracicaba, Brazil;* [2]*ESALQ, Piracicaba, Brazil*

ThP 253 **Single-Filament Imaging Mass Spectrometry-based Lipidomics in *Arthrospira platensis***; Lieve M. Laurens[1]; Peter V. Shanta[1]; Steven M Rowland[1]; [1]*National Renewable Energy Laboratory, Golden, CO*

ThP 254 **DESI-MS Imaging and the World of Extractables and Leachables on Glass Screens: Looking for Residue that Shouldn't Even Be There**; Samuel Merenbloom[1]; Wanda J Walczak[2]; [1]*Corning Incorporated, Painted Post, 14870;* [2]*Corning Incorporated, Painted Post, New York*

ThP 255 **Novel Tissue Washing Procedure for the Removal of Cation Adducts Prior to Selective Cation Formation for DESI and MALDI Imaging**; Mark Towers[1]; Lisa Reid[1]; Emmanuelle Claude[1]; [1]*Waters Corporation, Wilmslow, United Kingdom*

ThP 256 **A Multimodal Approach Using DESI-MSI and Laser Capture Microdissection for Single Tissue Section Analysis**; Emine Kazanc[1]; Evdoxia Karali[2]; Vincen Wu[1]; James Mckenzie[1]; Olof Isberg[1]; Andreas Dannhorn[1]; Paolo Inglese[1]; Sadaf Ghaem-Maghami[3]; George Poulogiannis[2]; Zoltan Takats[1]; [1]*Imperial College London, Department of Surgery and Cancer, United Kingdom;* [2]*Institute of Cancer Research, Division of Cancer Biology, United Kingdom;* [3]*Imperial College London, Hammersmith Hospital, London, United Kingdom*

ThP 257 **High Spatial Resolution Imaging in Endometrial Carcinoma Using Nanospray Desorption Electrospray Ionization Mass Spectrometry**; Ruichuan Yin[1]; Kristin Burnum-Johnson[2]; Xiaofei Sun[3]; Sudhansu K. Dey[3]; Julia Laskin[1]; [1]*Department of Chemistry, Purdue University, West Lafayette, IN;* [2]*Pacific Northwest National Laboratory, Richland, WA;* [3]*Division of Reproductive Sciences, Cincinnati Children's Hospital Medical Center, Cincinnati, OH*

ThP 258 **Three-Dimensional (3D) Imaging with Infrared Matrix-Assisted Laser Desorption Electrospray Ionization (IR-MALDESI) Mass Spectrometry**; Hongxia Bai[1]; Sitora Khodjaniyazova[1]; Theresse M. Robinson[1]; Kenneth P. Garrard[1,2]; David C Muddiman[1,3]; [1]*North Carolina State University, Raleigh, NC;* [2]*Precision Engineering Consortium, North Carolina State University, Raleigh, NC;* [3]*Molecular Education, Technology, and Research Innovation Center (METRIC), North Carolina State University, Raleigh, NC*

ThP 259 **Infrared MALDESI Mass Spectrometry Imaging Reveals Details of the *Bradyrhizobium diazoefficiens*:Glyine Max (Soybean) Root Nodule Metabolome**; James A. Langston[1]; Cassandra Marin[2]; Måns Ekelöf[3]; J. Jacob Parnell[2]; [1]*Novozymes, Inc., Davis, CA;* [2]*Novozymes North America, Durham, NC;* [3]*North Carolina State University, Raleigh, NC*

ThP 260 **Direct Analysis of Bone Tissues Using Matrix-Assisted Laser Desorption Electrospray Ionization (MALDESI) Mass Spectrometry Imaging**; Sitora Khodjaniyazova[1]; Kenneth P. Garrard[1,2]; Nicholas J. Hanne[3]; Jacqueline H. Cole[3]; David C. Muddiman[1,4]; *[1]FTMS Laboratory for Human Health Research, Department of Chemistry, North Carolina State University, Raleigh, NC; [2]Precision Engineering Consortium, North Carolina State University, Raleigh, NC; [3]Joint Department of Biomedical Engineering, North Carolina State University and University of North Carolina at Chapel Hill, Raleigh, NC; [4]Molecular Education, Technology, and Research Innovation Center (METRIC), North Carolina State University, Raleigh, NC*

ThP 261 **Single Cell Classification of Cancerous Tissue Images using Multiplexed Ion Beam Imaging**; Jay G Tarolli[1]; Rachel Finck[1]; Murat Aksoy[1]; Jessica Finn[1]; Jason Ptacek[1]; *[1]IONpath, Menlo Park, CA*

ThP 262 ***In-situ* Nanoscale Chemical Characterization of Polymer Coating Melting and Crystallization *via* Multimodal Chemical Imaging**; Anton Ievlev[1]; Matthias Lorenz[1,2]; Olga S Ovchinnikova[3]; *[1]Oak Ridge National Laboratory, Oak Ridge, TN; [2]University of Tennessee, Knoxville, Knoxville, TN; [3]Oak Ridge National Laboratory, Oak Ridge, Tennessee*

ThP 263 **Tandem MS Imaging of (Sub-)Monolayer Coatings at High Spatial Resolving Power for Process Assessment in Device Fabrication**; Gregory L Fisher; *Physical Electronics, Chanhassen, MN*

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ThP 264 **Comparative Study of Multiple Omics Data with or without Sonication in CPTAC Optimized Proteomic Protocol**; Tung-shing M Lih[1]; David J. Clark[1]; Lijun Chen[1]; Michael Schnaubelt[1]; Hui Zhang[1]; *[1]Johns Hopkins University School of Medicine, Baltimore, MD*

ThP 265 **Providing Local and Cloud Pipeline Support for Data Analysis with Skyline in the Context of PanoramaWeb Using Uber cadence Framework**; Joshua Aldrich[1]; Austin Keller[1]; Jarrett Egertson[1]; Josh Eckels[2]; Brendan X MacLean[1]; Micheal J MacCoss[1]; *[1]University of Washington, Seattle, WA; [2]LabKey, San Diego, CA*

ThP 266 **DIASibling: Learning to Detect Sibling Peptide Pairs in Data Independent Acquisition Mass Spectrometry Data**; Yang Lu[1]; Ricard Rodriguez[1]; Judit Villen[1]; William Stafford Noble[1]; *[1]University of Washington, Seattle, WA*

ThP 267 **DPHL: A Computational MS/MS Data Resource Enabling Robust Protein Biomarker Discovery using Data-Independent Acquisition and Parallel Reaction Monitoring**; Tiansheng Zhu[1,2,3]; Yi Zhu[1,2]; Yue Xuan[4]; Ruedi Aebersold[5]; Connie R. Jimenez[6]; Tiannan Guo[1,2]; *[1]School of Life Sciences, Westlake University, China, Hangzhou, China; [2]Institute of Basic Medical Sciences, Westlake Institute for Advanced Study, China, Hangzhou, China; [3]School of Computer Science, Fudan University, Shanghai, China; [4]ThermoFisher Scientific (BREMEN) GmbH, Hanna-Kunath-Str 11, 28199 Bremen,, Bremen, Germany; [5]Department of Biology, Institute for Molecular Systems Biology, ETH Zurich, Zurich, Swaziland; [6]OncoProteomics Laboratory, Dept. of Medical Oncology, Cancer Center Amsterdam, VU University Medical Center, Amsterdam, The Netherlands, Amsterdam, Netherlands*

ThP 268 **Boosting PRM Based Targeted Proteomics Using SpectroDive**; Tejas Gandhi[1]; Oliver M. Bernhardt[1]; Sebastian Müller[1]; Ian Lienert[1]; Magdalena Bober[1]; Claudia Escher[1]; Lukas Reiter[1]; *[1]Biognosys AG, Schlieren, Switzerland*

ThP 269 **Direct Scoring from DIA Data Using High Connected Data Models**; Fras Wasim[1]; Cristiano Viega[1]; Stephen A Tate[1]; *[1]SCIEX, Concord, ON*

ThP 270 **Enhanced Scoring of DIA Data Extraction Using Machine Learning**; Gillian Brooks[1]; Fras Wasim[1]; Stephen A Tate[1]; *[1]SCIEX, Concord, ON*

ThP 271 **artMS: Analytical R Tools for Mass Spectrometry**; David Jimenez-Morales[1]; John Von Dollen[2]; Alexandre Rosa Campos[3]; Nevan Krogan[2]; Danielle Swaney[2]; *[1]Stanford University, Stanford, CA; [2]UCSF, San Francisco, CA; [3]Sanford Burnham Prebys Medical Discovery Institute, La Jolla, CA*

ThP 272 **DIA-Only Chromatogram Libraries Made from Deep Neural Network MS2 Modeling Outperform Sample-Specific DDA Libraries**; Brian C. Searle[1,2]; Tobias Schmidt[3]; Siegfried Gessulat[3]; Bernhard Kuster[3]; Mathias Wilhelm[3]; *[1]Institute for Systems Biology, Seattle, Washington; [2]Proteome Software Inc., Portland, OR; [3]Technical University of Munich, Freising, Germany*

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ThP 273 **Recent Developments in the Multi-Level Structures for Lossless Ion Manipulations**; Adam Hollerbach[1]; Aneesh Prabhakaran[1]; Ailin Li[1]; Sandilya Garimella[1]; Randolph V. Norheim[1]; Colby E. Schimelfenig[1]; Richard D. Smith[1]; Yehia M Ibrahim[1]; *[1]Pacific Northwest National Laboratory, Richland, WA*

ThP 274 **Carbohydrate Isomer Separations with Multiple Ion Mobility-Mass Spectrometry Platforms**; Kristin R. McKenna[1,2]; Li Li[1,2]; Zhao Li[1,2]; Kelsey A. Morrison[3]; Ramanarayanan Krishnamurthy[2,4]; Charles L. Liotta[1,2]; Brian H. Clowers[3]; Facundo M Fernandez[1,2]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]Center for Chemical Evolution, Atlanta, GA; [3]Washington State University, Pullman, WA; [4]The Scripps Research Institute, La Jolla, CA*

ThP 275 **A New Bench-Top Dispersive Ion Mobility Spectrometer for Characterizing Biotherapeutic Drugs**; Henry Benner[1]; Ben Aguilar[1]; *[1]Ion Dx, Monterey, CA*

ThP 276 **The Development of a Natural Products Library Using Ion-Mobility Enabled Mass Spectrometry**; Jeff Goshawk[1]; Gitte Barknowitz[1]; Michael McCullagh[1]; *[1]Waters Corporation, Wilmslow, United Kingdom*

ThP 277 **Collision Induced Unfolding Captures Disease Relevant Differences in Stability and Ligand Binding for the Integral Membrane Peripheral Myelin Protein**; Sarah M. Fantin[1]; Kristine F. Parson[1]; Pramod Yadav[2]; Charles R. Sanders[3]; Melanie D. Ohi[2,4]; Brandon T. Ruotolo[1]; *[1]Department of Chemistry, University of Michigan, Ann Arbor, MI; [2]Life Sciences Institute, University of Michigan, Ann Arbor, MI; [3]Department of Biochemistry, Vanderbilt University, Nashville, TN; [4]Department of Cell and Developmental Biology, University of Michigan, Ann Arbor, MI*

ThP 278 **Evaluation of Ion Mobility-Assisted Data Independent Acquisition (UDMSE) for Metaproteomics Sample Analysis**; Lisa M Wolfe[1]; Kitty J. Brown[1]; Brad J Williams[2]; Giorgis Isaac[3]; Jessica E. Prenni[1,4]; Corey D. Broeckling[1]; *[1]Proteomics & Metabolomics Facility, Colorado State University, Fort Collins, CO; [2]Waters Corporation, Beverly, MA; [3]Waters Corporation, Milford, MA; [4]Department of Horticulture & Landscape Architecture, Colorado State University, Fort Collins, CO*

ThP 279 **Trapped Ion Mobility-Mass Spectrometry as Tool for Rapid Identification of Metal Binding Sites in Proteins**; Philipp Strohmidel[1]; Jens Fangmeyer[1]; Tilo D. Schachel[1]; Michael Sperling[1,2]; Uwe Karst[1]; *[1]University of Muenster, Institute of Inorganic and Analytical Chemistry, Muenster, Germany; [2]European Virtual Institute for Speciation Analysis (EVISA), Muenster, Germany*

ThP 280 **LC-MS with SelexION® Differential Mobility Separation Technology as a Sensitive and Selective Tool to Verify**

Quality of Olive Oil; Akanksha Singh[1]; Axel Besa[2]; Dipankar Malakar[1]; Manoj G Pillai[1]; *[1]SCIEX, Gurgaon, India; [2]SCIEX, Darmstadt, Germany*

ThP 281 **Effective Liquid Chromatography – Trapped Ion Mobility Spectrometry – Mass Spectrometry Separation of Isomeric Lipid Species**; Kevin Jeanne Dit Fouque[1]; Cesar E Ramirez[1]; Russell L Lewis[2]; Jeremy P Koelmel[2]; Timothy J. Garrett[2]; Richard A Yost[2]; Francisco A. Fernandez-Lima[1]; *[1]Florida International University, Miami, FL; [2]University of Florida, Gainesville, FL*

ThP 282 **Monitoring Protomer-Specific "Pin-Pong Effect" by Ion-Mobility Mass Spectrometry**; Athula B. Attygalle[1]; Zhaoyu Zheng[2]; *[1]Stevens Institute of Technology, Hoboken, NJ; [2]Stevens Institute of Tecnology, Hoboken, NJ*

ThP 283 **Characterization of the Intrinsically Disordered AT-Hook Peptides Using Mobility-Selected MS/MS and Action Infrared Spectroscopy**; Jacob Porter[1]; Phillip Maitre[2]; Fenfei Leng[1]; Francisco Fernandez-Lima[1]; *[1]Florida International University, Miami, FL; [2]Université Paris-Sud, Orsay, France*

ThP 284 **Conformation Dynamics of CRISPR/Cas9 Binding with sgRNA Studied by Native MS and IM-MS**; Defu Wang; *NJUST, Nanjing, China*

ThP 285 **Application of Cyclic Ion Mobility Coupled to Mass Spectrometry for High Peak Capacity Analysis of Native and Deuterated Peptide Mixtures**; Martin Palmer[1]; Malcolm Anderson[1]; Dale Cooper-Shepherd[1]; James I Langridge[1]; Robert Tonge[1]; John R. Engen[2]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Northeastern University, Boston, MA*

ThP 286 **Unravelling Macrocycle Conformational Space and Self-Assembly Using Ion-Mobility Mass Spectrometry and Distance Geometry Modeling**; Thanh D Do[1]; MD Ashraful Haque[1]; *[1]University of Tennessee, Knoxville, Knoxville, TN*

ThP 287 **Structural Study of Analogues of Titan's Haze by Trapped Ion Mobility Coupled with a Fourier Transform Ion Cyclotron Mass Spectrometer**; Christopher Paul Rüger[1]; Julien Maillard[1,2]; Johann Le Maître[1,3]; Mark E. Ridgeway[4]; Christopher J. Thompson[4]; Isabelle Schmitz-Afonso[1]; Thomas Gautier[2]; Nathalie Carrasco[2]; Melvin A. Park[4]; Pierre Giusti[3]; Carlos Afonso[1]; *[1]Normandy University, COBRA laboratory, Mont Saint Aignan, France; [2]LATMOS/IPSL, UVSQ Université Paris-Saclay, Paris, France; [3]Total Research & Technology Gonfreville, Harfleur, France; [4]Bruker Daltonics Inc., Billerica, MA*

ThP 288 **Investigation of Cationized Steroid Dimer Formation by Ion Mobility-Mass Spectrometry for Improved Analysis of Anabolic Androgenic Steroids in Anti-Doping Testing**; Allison Levy[1]; Richard A Yost[1]; *[1]University of Florida, Gainesville, FL*

ThP 289 **Elucidating Protein Structure Using High Resolution Ion Mobility-Orbitrap**; Jacob W McCabe[1]; Michael L Poltash[1]; Mehdi Shirzadeh[1]; Arthur Laganowsky[1]; David H. Russell[1]; *[1]Texas A&M University, College Station, TX*

ThP 290 **Improving Structure Elucidation in Metabolomics Analyses with Ion Mobility and Multiple Fragmentation Methods**; Samuel Maddox[1]; Kristie Baker[1]; Robert Fraser Caris[1]; Roba Alzahrani[1]; Reda Massawe[1]; Christopher D. Chouinard[1]; *[1]Florida Institute of Technology, Melbourne, FL*

ThP 291 **Development of Separation Method of Metabolic Isomers Using Ion Chromatography-Differential Mobility Spectrometry-Mass Spectrometry**; Akiyoshi Hirayama[1]; Tomoyoshi Soga[1]; *[1]Institute for Advanced Biosciences, Keio University, Tsuruoka, Japan*

ThP 292 **Development of Native Ion Mobility Spectrometry-Mass Spectrometry with Extended 20k Mass Range for Intact Proteins and Intact Protein Complexes**; Xueyun Zheng[1]; Ruwan T. Kurulugama[2]; Sandy Yates[2]; John Sausen[2]; Arthur Laganowsky[1]; David H. Russell[1]; *[1]Department of Chemistry, Texas A&M University, College Station, TX; [2]Agilent Technologies, Inc., Santa Clara, CA*

ThP 293 **Gas-Phase Unfolding Reveals Subtle Stability Shifts in Higher-Order Substrate-Cytochrome P450 Complexes**; Chunyi Zhao[1]; Kinshuk Srivastava[2]; David Sherman[1,2]; Brandon T. Ruotolo[1]; *[1]Department of Chemistry, University of Michigan, Ann Arbor, MI; [2]Life Sciences Institute, University of Michigan, Ann Arbor, MI*

ThP 294 **Separation of Isomeric and Isobaric Oligonucleotides by Ion Mobility Mass Spectrometry**; Asha Hewarathna[1]; Kui Yang[1]; Connie Ruzicka[1]; David Keire[1]; *[1]US FDA, St. Louis, MO*

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ThP 295 **Mobility Calibration of Trapped Ion Mobility Spectrometry -Mass Spectrometry Experiments**; Kim Q. Dang[1]; Kevin Jeanne Dit Fouque[1]; Francisco Fernandez-Lima[1]; *[1]FIU, Miami, FL*

ThP 296 **Assessing Collision Cross Section Calibration Strategies in Structures for Lossless Ion Manipulations (SLIM)**; Ailin Li[1]; Daniel J. Orton[1]; Kent J. Bloodsworth[1]; Randolph V. Norheim[1]; Colby E. Schimelfenig[1]; Richard D. Smith[1]; Yehia M. Ibrahim[1]; *[1]PNNL, Richland, WA*

ThP 297 **Chemical Modification and Cluster Dynamics in High Kinetic Energy IMS (HiKE-IMS)**; Florian Stappert[1]; Maria Allers[2]; Duygu Erdogdu[1]; Ansgar T. Kirk[2]; Walter Wissdorf[1]; Hendrik Kersten[1]; Stefan Zimmermann[2]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany; [2]Leibniz University Hannover, Hannover, Germany*

ThP 298 **Improving Ion Mobility – Mass Spectrometry Performance Using a Tristate Ion Shutter with Extremely Low Ion Discrimination**; Ansgar T. Kirk[1]; Tobias Reinecke[2]; Cornelius Wendt[1]; Pearl Kwantwi-Barima[2]; Christian Thoben[1]; Brian H. Clowers[2]; Stefan Zimmermann[1]; *[1]Institute of Electrical Engineering and Measurement Technology, Department of Sensors and Measurement Technology, Leibniz University Hannover, Hannover, Germany; [2]Department of Chemistry, Washington State University, Pullman, WA*

ThP 299 **Simulation of Cluster Dynamics in High Kinetic Energy IMS (HiKE-IMS)**; Duygu Erdogdu[1]; Maria Allers[2]; Ansgar T. Kirk[2]; Florian Stappert[1]; Walter Wissdorf[1]; Hendrik Kersten[1]; Stefan Zimmermann[2]; Thorsten Benter[1]; *[1]University of Wuppertal, Wuppertal, Germany; [2]Leibniz University Hannover, Hannover, Germany*

ThP 300 **Analysis of Collision Cross Sections for the Potassium Cation in Rare Gases using Simplified Classical/Semi-classical Collision Theory**; Glenn E. Spangler; *Technispan LLC, Lutherville, MD*

ThP 301 **Ion Compaction in Native Ion Mobility-Mass Spectrometry: a Comparison of Molecular Dynamics Force Fields**; Amber D Rolland[1]; Daniel Ko[1]; James S Prell[1]; *[1]University of Oregon Department of Chemistry and Biochemistry, Eugene, OR*

ThP 302 **Resolution and Characterisation of Protomer and Radical Cation Species Utilising a Cyclic Ion Mobility-Enabled Quadrupole Time-of-Flight (Q-cIM-oaToF) Mass spectrometer**; James Scrivens[1]; Gillian Taylor[1]; Martin Palmer[2]; Jakub Ujma[2]; Kevin Giles[2]; Jonathan P Williams[2]; *[1]Teesside University, Middlesbrough, United Kingdom; [2]Waters Corportaion, Cheshire, United Kingdom*

ThP 303 **Evaluation of a Modular Atmospheric Pressure Drift Tube Coupled to an Orbitrap™ Mass Spectrometer with Ultraviolet Photodissociation for Biomolecule Analysis**; James D Sanders[1]; Sarah Sipe[2]; Tobias Reinecke[3]; Brian H. Clowers[3]; Jennifer S Brodbelt[2]; *[1]University of Texas, Austin, Austin, TX; [2]University of Texas at Austin, Department of Chemistry, Austin, TX; [3]Washington State University, Department of Chemistry, Pullman, WA*

ThP 304 **Portable High Resolution Periodic Focusing Differential Mobility Analyzer;** Kent Gillig[1]; Guan-Bo Liao Liao[1]; Da-Shung Su[1]; Chi-Huang Huang[1]; Yuri A. Dyakov[1]; Feng-Wen Jiang[1]; Chung-Hsuan Chen[1]; *[1]Academia Sinica, Taipei, Taiwan*

ThP 305 **Pseudo-Trapping within Traveling Wave Ion Guides: Discovery and Implications for Ion Mobility Separations;** Sugyan M. Dixit[1]; Keith Richardson[2]; David Langridge[2]; Kevin Giles[2]; Brandon T. Ruotolo[1]; *[1]University of Michigan, Ann Arbor, MI; [2]Waters Corporation, Wilmslow, United Kingdom*

ThP 306 **Dendrimer Calibrations for Ion Mobility-Mass Spectrometry;** Scott M. Grayson[1]; Michael Malkoch[2, 3]; Jamie Godfrey[2]; Charlotte Mooney[4]; Perdita E. Barran[4]; Nick Tomczyk[5]; Kevin Giles[5]; *[1]Tulane University, New Orleans, LA; [2]Polymer Factory Sweden AB, Stockholm, Sweden; [3]KTH Royal Institute of Technology, Stockholm, Sweden; [4]The University of Manchester, Manchester, United Kingdom; [5]Waters Corporation, Wilmslow, United Kingdom*

ThP 307 **Conformational Diversity of Vasotocin Nonapeptide Diastereomers Revealed by Uniform Field and Cyclic Traveling Wave Ion Mobility-Mass Spectrometry Measurements;** Shawn T. Phillips[1]; Emanuel Zlibut[1]; Jody C. May[1]; John A. McLean[1]; Martin E. Palmer[2]; Dale A. Cooper-Shepherd[2]; James I. Langridge[2]; *[1]Vanderbilt University, Nashville, TN; [2]Waters Corporation, Wilmslow, United Kingdom*

ThP 308 **Molecular Classification and Identification Using Tandem Ion Mobility Spectrometry with Neural Networks Analysis of Mobility Selected Ions and Full Spectra;** Hossein Shokri[1]; Natividad Jurado-Campos[2]; Ben Gardner[3]; Niu Hsein-Chi W[4]; Erkinjon Nazarov[1]; Gary A. Eiceman[1]; *[1]New Mexico State University, Las Cruces, NM 88003; [2]University of Córdoba, Rabanales, Spain; [3]Collins Aerospace, 960 Overland Court, San Dimas, CA; [4]960 Overland Court, San Dimas, CA*

ThP 309 **Effects of Solvent and Source Temperature on Ion Mobility Collision Cross Section Measurements;** Nadjali Chung[1]; Jody C. May[1, 2]; Renã A.S. Robinson[1]; John A. McLean[1, 2]; *[1]Vanderbilt University Department of Chemistry, Nashville, TN; [2]Center for Innovative Technology, Nashville, TN*

ThP 310 **Blanc's Law for the ESI Era: Predicting Ion Mobility in Mixed Drift Gases;** Cameron N. Naylor[1]; Tobias Reinecke[1]; Mark E. Ridgeway[2]; Melvin A. Park[2]; Brian H. Clowers[1]; *[1]Washington State University, Department of Chemistry, Pullman, WA; [2]Bruker Daltonics Inc., Billerica, MA*

ThP 311 **Leveraging Ion-Vapor Induced Mobility Shifts to Deduce Gibbs Free Energies of Association for Alcohols and Amino Acids;** Pearl Kwantwi-Barima[1]; Christopher J. Hogan[2]; Brian H. Clowers[1]; *[1]Washington State University, Pullman, WA; [2]Department of mechanical engineering, university of minnesota, Minneapolis, Minnesota*

ThP 312 **Monitoring Photoisomerization of Resveratrol by Ion–Mobility Mass Spectrometry (IM-MS);** Gabriella V. Litterio[1]; Sihang Xu[1]; Athula Attygalle[1]; *[1]Stevens Institute of Tecnology, Hoboken, NJ*

ThP 313 **The Effect of High Fields and Strong Dipole Moments on Ion Mobility and Collision Cross Sections;** Carlos Larriba Andaluz[1]; Tianyang Wu[1, 2]; *[1]IUPUI, Indianapolis, IN; [2]Purdue University, West Lafayette, IN*

ThP 314 **Efficient Trapping, Storage, and Utilization of Ions With On-Board Accumulation in Structures for Lossless Ion Manipulations;** Liulin Deng[1]; Daniel DeBord[1]; Ahmed M Hamid[1]; Kelly L. Wormwood[1]; Anisha Yadav[1]; Gregory Webster[1]; Gordon A Anderson[2]; *[1]MOBILion Systems Inc., Exton, PA; [2]GAA Custom Engineering, LLC, Benton City, WA*

ThP 315 **Practical Two-Dimensional High-Resolution Ion Mobility Separations by Combining FAIMS with Trapped IMS;** Jacob Porter[1]; Kevin Jeanne Dit Fouque[1]; Francisco A. Fernandez-Lima[1]; Alexandre A. Shvartsburg[2]; *[1]Florida International University, Miami, FL; [2]Wichita State University, Wichita, KS*

ThP 316 **Predicting Ion Mobility Spectra Using Gas Phase Molecular Dynamics (MD) in Combination of Projection Superposition Approximation (PSA) Algorithm;** Tyler C. Cropley[1]; Mengqi Chai[1]; Fanny C. Liu[1]; Albert Konijnenberg[2]; Rani Moons[2]; Frank Sobott[2]; Christian Bleiholder[1]; *[1]Florida State University, Tallahassee, FL; [2]University Of Antwerp, Antwerp, Belgium*

ThP 317 **Characterization and Optimization of the m/z Transmission and Resolution of Structures for Lossless Ion Manipulations (SLIM);** Ahmed Mohamed Hamid[1]; Liulin Deng[1]; John Daniel DeBord[1]; Kelly Wormwood[1]; Anisha Yadav[1]; Gregory Webster[1]; Gordon A Anderson[2]; *[1]MOBILion Systems Inc., Exton, PA; [2]GAA Custom Engineering, LLC, Benton, WA*

ThP 318 **Differentiation of Aspartic Acid and Isoaspartic Acid Isomeric Peptides with Drift Tube Ion Mobility Spectrometry;** Karen E. Butler[1]; James N. Dodds[1]; Erin S. Baker[1]; *[1]North Carolina State University, Raleigh, NC*

ThP 319 **An Improved Calibration Approach for Travelling Wave Ion Mobility Spectrometry: Robust, High-precision Collision Cross Sections;** Keith Richardson[1]; David Langridge[1]; Sugyan M. Dixit[2]; Kevin Giles[1]; Brandon T. Ruotolo[2]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Department of Chemistry, University of Michigan, Ann Arbor, MI*

ThP 320 **Introducing Structural Detail in Ion Mobility Spectra of Alcohols at Ambient Pressure Using a Tandem Drift Tube with Reactive Stage;** Hossein Shokri[1]; Maika Vuki[2]; Ben Gardner[3]; Niu Hsein-Chi W[4]; Umesh Chiluwal[1]; Bhupendra Gurung[1]; David Emery[1]; Gary A. Eiceman[1]; *[1]New Mexico State University, Las Cruces, NM, 88003; [2]University of Guam, Mangilao, Guam, 96923; [3]Collins Aerospace, 960 Overland Court, San Dimas, CA; [4]960 Overland Court, San Dimas, CA*

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ThP 321 **Measurement of Myc Synthesis Using a Stable Isotope Tracer Method;** Haihong Zhou[1]; Natalie Daurio[1]; Mark Demma[1]; Claudio Mapelli[1]; Abbas Walji[1]; Ying Chen[1]; David McLaren[1]; Stephen Previs[1]; Jennifer O'Neil[1]; *[1]Merck Inc. & Co., Kenilworth, NJ*

ThP 322 **13C-Metabolic Flux Analysis of Inhibitor-Induced Metabolic Redirection in the Central Metabolism of Breast Cancer Cells;** Fumio Matsuda[1]; Chie Araki[1]; Kousuke Maeda[1]; Nobuyuki Okahashi[1]; Hiroshi Shimizu[1]; *[1]Osaka University, Suita, Japan*

ThP 323 **Automated Mass Isotopologue Distribution Analysis for Metabolic Flux Quantification of Lipids in Cells Treated with Xanthohumol;** Ines L Paraiso[1]; Jaewoo Choi[1]; Claudia S. Maier[2]; Jan F. Stevens[1]; *[1]Linus Pauling Institute, College of Pharmacy, Oregon State University, Corvallis, OR; [2]Department of Chemistry, Oregon State University, Corvallis, OR*

ThP 324 **Defining the Immune-Modulatory Actions of Electrophilic Fatty Acids Using 13C flux;** Steven J Mullett[1]; Greg J Buchan[1]; James P O'Brien[1]; Crystal Uvalle[1]; Stacy Gelhaus Wendell[2]; *[1]University of Pittsburgh, Pittsburgh, PA; [2]Univ of Pittsburgh, Pittsburgh, PA*

ThP 325 **Increased Multiplexing of DiLeu Isobaric Tags with Enhanced Linker Using Mass Defect Isotope Encoding;** Dustin Frost[1]; Ting-Jia Gu[1]; Miyang Li[2]; Feng Yu[1]; Lingjun Li[1]; *[1]School of Pharmacy, University of Wisconsin-Madison, Madison, WI; [2]Department of Chemistry, University of Wisconsin, Madison, WI*

ThP 326 **Top-Down Analysis of Intact Protein Derived Immonium Isotopologue Ions Provides an Improved Strategy for Measuring Proteoform Turnover**; Thomas Angel[1]; Matthew E Szapacs[1]; *[1]GSK, Collegeville, PA*

ThP 327 **Stable Isotope-Resolved Metabolomics under Pharmacologically Controlled Metabolic States**; Pawel Lorkiewicz[1]; Andrew Gibb[2]; Benjamin Rood[1]; Liqing He[1]; Yuting Zheng[1]; Xiang Zhang[1]; Bradford Hill[1]; *[1]University of Louisville, Louisville, KY; [2]Temple University, Philadelphia, PA*

ThP 328 **Automated High-Throughput Flux Analysis of Non-Small Cell Lung Carcinoma Cells Grown *in vitro* in Two and Three Dimensions**; David Heywood[1]; Suraj Dhungana[2]; Johannes PC Vissers[1]; Abhishek Jha[3]; Raghav Sehgal[3]; Amrita Cheema[4]; *[1]Waters Corporation, Wilmslow, United Kingdom; [2]Waters Corporation, Milford, MA; [3]Elucidata, Cambridge, MA; [4]Georgetown University, Washington, DC*

ThP 329 **Identifiability and Tracer Selection in Metabolic Flux Analysis**; Xiaoyang Su[1]; Chi Song[2]; *[1]Rutgers University, New Brunswick, NJ; [2]The Ohio State University, Columbus, OH*

ThP 330 **Ultrahigh Resolution MS3 by UV Photodissociation can Reveal Unprecedented Detail of Pathways under Stable Isotope Resolved Metabolomics (SIRM)**; Richard Higashi[1,2,3]; Woo-Young Kang[1]; Teresa W-M. Fan[1,2,3]; Andrew N. Lane[1,2,3]; *[1]Center for Environmental and Systems Biochemistry, University of Kentucky, Lexington KY, Lexington, Kentucky; [2]Markey Cancer Center, University of Kentucky, Lexington, Kentucky; [3]Dept. of Toxicology and Cancer Biology, University of Kentucky, Lexington, Kentucky, United States, Lexington, KY*

ThP 331 **Isotopic 13C Enrichment in Multimer Ion Adducts of Intracellular Metabolites for Potential Applications in 13C Metabolic Flux Analysis**; Charulata B. Prasannan[1,2]; Vivek Mishra[1]; Damini Jaiswal[1]; Pramod P. Wangikar[1,2,3]; *[1]Department of Chemical Engineering,Indian Institute of Technology Bombay, Mumbai, India; [2]DBT-Pan IIT Center for Bioenergy, Indian Institute of Technology Bombay, Mumbai, India; [3]Wadhwani Research Center for Bioengineering, Indian Institute of Technology Bombay, Mumbai, India*

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ThP 332 **An LC-MS/MS-Based Analytical Method for Separation and Quantitative Analysis of Marfey's Reagent Derivatized Proteinogenic Amino Acids dl-Stereoisomers**; Navid J. Ayon[1]; Amar D. Sharma[1]; William G. Gutheil[1]; *[1]University of Missouri-Kansas City, Kansas City, MO*

ThP 333 **An Alternative Narrow-Bore Column to Facilitate High-Throughput "UHPLC" Type and microflow LC-MS Strategies for Residue Analysis**; Arianne Soliven[1]; Lucia Pareja[2]; Horacio Heinzen[1]; Andrés Pérez Parada[1,3]; *[1]Grupo de Analisis de Compuestos Traza, Facultad de Química, Universidad de la Republica,, Montevideo, Uruguay; [2]Departamento de Química del Litoral, CENUR LO, Universidad de la República, Paysandú, Uruguay; [3]Departamento de Desarrollo Tecnológico, CURE, Universidad de la República, Rocha, Uruguay*

ThP 334 **Optimization and Automated Selection of Assigned Charge States for Therapeutic Peptide Bioanalysis**; Mary Piotrowski[1]; Wayne Lootsma[2]; Julie Keefer[1]; Hui Zhang[1]; Joseph Janiszewski[2]; Steve Ainley[2]; *[1]Pfizer, Groton, CT; [2]Sound Analytics, Niantic, CT*

ThP 335 **Multiplexing Independent Streams to Increase LC/MS/MS Throughput**; Mary A Piotrowski[1]; Brendon Kapinos[1]; Julie Keefer[1]; Steven S Gernhardt[1]; Hui Zhang[1]; Wayne Lootsma[2]; Steve Ainley[2]; *[1]Pfizer, Groton, CT; [2]Sound Analytics, Niantic, CT*

ThP 336 **Robust Extraction, Separation and Quantitation of Structural Isomer Steroids From Human Plasma by SPE with LC-MS/MS Detection**; Jon Bardsley[1]; Kean Woodmansey[1]; Tim Liddicoat[1]; Stacy Tremintin[1]; *[1]Thermo Fisher Scientific, Tudor Road, United Kingdom*

ThP 337 **Establish an Analytical Model for Chemical Preservatives Using QTOF and MPP software**; Shaozhen Wang; *Agilent Technologies, Shanghai, China*

ThP 338 **Hydrogen-Deuterium Exchange Liquid Chromatography / High Resolution Mass Spectrometry for Structure Elucidation of Unknown Organic Molecules**; Chengli Zu[1]; Renzo Samame[1]; Daniel Knueppel[1]; Jeffery Gilbert[1]; *[1]Corteva Agriscience, Indianapolis, IN*

ThP 339 **High Resolution Mass Spectrometry with Automated Data Analysis to Support Structural Elucidation of Degradation Impurities of Drug Molecules**; Yuejie Zhao[1]; Yong Liu[1]; Blanca Serra[2]; Elisabeth Ortega-Carrasco[2]; Ismael Zamora[2]; Kevin P. Bateman[3]; *[1]Merck & Co., Inc., Rahway, NJ; [2]Lead Molecular Design, S.L., Sant Cugat Del Valles, Spain; [3]Merck & Co., Inc., West Point, PA*

ThP 340 **Automatic Detection of Impurities and Byproducts in Complicated Reactions Using LC-HRMS**; Elisabeth Ortega-Carrasco[1]; Jenny Desantis[2]; Fabien Fontaine[1]; Blanca Serra[1]; Paolo Benedetti[3]; Ismael Zamora[1,3]; *[1]Lead Molecular Design, S.L., Sant Cugat Del Valles, Spain; [2]University of Perugia, Perugia, Italy; [3]Molecular Discovery, London, United Kingdom*

ThP 341 **An Integrated Approach for the Estimation of Hazardous Transformation Products from Metoprolol and Metoprolol Acid in UV/H2O2 Treated Waste Waters**; Adrian Jaen-Gil[1]; Gianluigi Buttiglieri[1]; Aleix Benito[2]; Rafael Gonzalez-Olmos[2]; Sara Rodriguez-Mozaz[1]; Damia Barcelo[1]; *[1]ICRA, Girona, Spain; [2]IQS School of Engineering, Universitat Ramon Llull, Barcelona, Spain*

ThP 342 **Multiple Ion Transition Summation of Isotopologues for Improved Mass Spectrometric Detection of N-Acetyl-S-(1,2-dichlorovinyl)-L-cysteine, a Biomarker of Exposure to Trichloroethylene**; Deepak Bhandari[1]; Cameron S. Movassaghi[2]; Benjamin C. Blount[2]; Víctor R. De Jesús[2]; *[1]Centers for Disease Control and Prevention, Atlanta, Ga; [2]Centers for Disease Control and Prevention, Atlanta, GA*

ThP 343 **Structural Analysis of Impurities in Pharmaceutical Ingredients Using Trap-Free 2D-LC High-Resolution Accurate Mass Spectrometry**; Tetsuo Iida[1]; Yusuke Inohana[1]; Tairo Ogura[1]; *[1]Shimadzu Corporation, Kyoto, Japan*

ThP 344 **A Versatile Hybrid HILIC and Ion Exchange Column for the Separation of a Wide Range of Polar Compounds**; Connor Flannery[1]; Vernon C. Bartlett[1]; Ahren Green[1]; Terry S. Reid[1]; Xiaoning Lu[1]; *[1]Restek, Bellefonte, PA*

ThP 345 **Retention Time Prediction for 653 Pesticides on a Biphenyl Liquid Chromatography Stationary Phase Using Machine Learning**; Anthony Sullivan[1]; Leon P Barron[2]; Alan Barnes[3]; Neil Loftus[3]; *[1]Shimadzu UK Limited, Milton Keynes, United Kingdom; [2]Department of Analytical, Environmental & Forensic Sciences, School of Population Health & Environmental Sciences, Faculty of Life Sciences and Medicine, King's College London, United Kingdom; [3]Shimadzu Corporation, Manchester, United Kingdom*

ThP 346 **Development of Two-Dimensional Supercritical Fluid Chromatography-Liquid Chromatography-Mass Spectrometry (2D-SFC-LC-MS) for Surfactants Analysis**; Yuka Fujito[1]; Masato Ohmine[2]; Hiroyasu Umemura[2]; Takuya Tsutsui[2]; Akinori Igarashi[2]; Yoshihiro Hayakawa[3]; *[1]Shimadzu Scientific Instruments, Inc., Columbia, Maryland; [2]Lion Corporation, Tokyo, Japan; [3]Shimadzu corp., Kyoto, Japan*

ThP 347 **Investigation into the Suitability of Coupling Direct Analyte-Probed Nanoextraction (DAPNe) to Liquid**

Chromatography Mass Spectrometry (LC-MS); Holly-May Lewis[1]; Roger Webb[1]; Janella de Jesus[1]; Catia Costa[1]; Vladimir Palitsin[1]; Josephine Bunch[2]; Guido Verbeck[3]; Melanie Bailey[1]; *[1]University of Surrey, Guildford, United Kingdom; [2]National Physical Laboratory, London, United Kingdom; [3]University of North Texas, Denton, TX*

ThP 348 **Efficient Identification and Management of Degradant Data in Process Development**; Anne Marie Smith[1]; Andrew Anderson[1]; Sanjivanjit K. Bhal[1]; Joe DiMartino[1]; *[1]ACD/Labs, Toronto, ON*

ThP 349 **Making Mass Spectrometry Analysis Easy and Automated by using Mass Hunter Walk Up Open Access Software**; Kyle J Covert[1]; Robert Ley[1]; *[1]Agilent Technologies, Inc., Santa Clara, CA*

ThP 350 **Improved Analysis Profiling of Organic Semiconductor Materials by High-Resolution Mass Spectrometry with Supercritical Fluid Chromatography**; Yunju Cho[1]; Keumjung Yoon[2]; Sunghwan Kim[1, 2]; *[1]Green-Nano Materials Research Center, Daegu, South Korea; [2]Kyungpook National University, Daegu, South Korea*

ThP 351 **Crown Chromatography: Cation-Binding Agents as Mobile Phase Additives in HILIC**; Taylor A. Harmon[1]; Richard A Yost[1]; Timothy Garrett[1, 2]; *[1]University of Florida Department of Chemistry, Gainesville, FL; [2]University of Florida Department of Pathology, Immunology, and Laboratory Medicine, Gainesville, FL*

ThP 352 **Application of 2D LC with MS Detection with Superficially Porous Columns to the Analysis of Cold Medicine**; William Long[1]; Anne E Mack[2]; Carl Griffin[2]; *[1]Agilent Technologies, Wilmington, DE; [2]Agilent Technologies, Inc., Wilmington, DE*

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ThP 353 **Assessing Contamination in Publicly Available Proteomic Datasets**; Matthew Rardin[1]; Daryl Bulloch[1]; Bradford W. Gibson[1]; *[1]Amgen, South San Francisco, CA*

ThP 354 **Systematic Structural Optimization of Mass Spec Compatible Surfactants for Proteomic Applications**; Valerie Ressler[1]; Wenhui Zhou[1]; Joel Walker[1]; Jean Osterman[1]; Sergei Saveliev[1]; Mike Rosenblatt[1]; Poncho Meisenheimer[1]; Marjeta Urh[1]; *[1]Promega Corporation, Madison, WI*

ThP 355 **On-Chip Digestion Coupled to Nano LC MS/MS**; Massamba Mbacké Ndiaye[1]; Giovanni Chiappetta[1]; Joêlle Vinh[1]; *[1]ESPCI - PSL, Paris, France*

ThP 356 **Streamlined Proteomic Profiling of Quantity-Limited Clinical Tissue Facilitated by Automated Sample Preparation and Mass Spectrometry**; Torsten Mueller[1]; Mathias Kalxdorf[2, 3]; Marcel Kool[2, 4]; Kristian W Pajtler[2, 4, 5]; Jeroen Krijgsveld[2, 6]; *[1]DKFZ, Heidelberg, Germany; [2]DKFZ, Heidelberg, Germany; [3]The European Molecular Biology Laboratory, Heidelberg, Germany; [4]NCT Heidelberg (KiTZ), Heidelberg, Germany; [5]Pediatric Oncology, Hematology and Immunology, University Hospital, Heidelberg, Germany; [6]Medical Faculty, Heidelberg University, Heidelberg, Germany*

ThP 357 **A Quick and Sensitive LC-MS/MSMethod for Quantitation of Intact Insulin Analogs in Rat and Human Plasma**; Dawei Zhou[1]; Sharon Tong[1]; *[1]WuXi AppTec, Cranbury, NJ*

ThP 358 **Comparison of Six Proteomics Sample Preparation Methods, Digestion Reagents and Proof of Principle Automation**; Aleksandr Gaun[1]; Sudha Gollapudi[1]; Rob Keyser[1]; Fiona McAllister[1]; *[1]Calico Labs, South San Francisco, CA*

ThP 359 **Comparison of Homogenization Techniques towards a Universal Method for the Analysis of Mouse Tissues Using Multiple Reaction Monitoring-Mass Spectrometry (MRM-MS)**; Helena Pětrošová[1]; Sarah A. Michaud[1]; Angela Jackson[1]; Nicholas J. T. Sinclair[1]; Christoph H. Borchers[1, 2, 3, 4]; *[1]University of Victoria-Genome BC Proteomics Centre, Victoria, BC; [2]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; [3]Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; [4]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC*

ThP 360 **Improving Host Cell Protein Profiling in Biopharmaceuticals by Advanced LC-MS/MS Methods**; Regina Kufer[1]; Martina Suessmair[1]; Ingo Lindner[1]; Don Walker[2]; Christopher Yu[2]; Stefanie Wohlrab[1]; Markus Haindl[1]; Harald Wegele[1]; *[1]Roche Diagnostics GmbH, Penzberg, Germany; [2]Genentech, South San Francisco, CA*

ThP 361 **A Method to Optimize Proteome Analyses of Low Cell Numbers of Pathogens Retrieved from Infection Assays**; Manuela Gesell Salazar[1]; Sascha Blankenburg[1]; Christian Hentschker[1]; Denise Dittmar[1]; Petra Hildebrandt[1]; Stephan Michalik[1]; Anna Nagel[1]; Kristin Surmann[1]; Uwe Völker[1]; *[1]University Medicine Greifswald, Greifswald, Germany*

ThP 362 **Kinetics of Acetone Precipitation: Investigation of Whether Protein Properties Influence the Rate of Precipitation under Various Solvent Conditions**; Jessica L. Nickerson[1]; Alan A. Doucette[1]; *[1]Dalhousie University, Halifax, NS*

ThP 363 **High Throughput Intact Glycopeptide Enrichment for Site-specific N-linked Glycosylation Analysis Utilizing Automated Liquid Handling Systems**; Shao-Yung Chen[1]; Ganglong Yang[1]; David J. Clark[1]; Hui Zhang[1]; *[1]Johns Hopkins University School of Medicine, Baltimore, MD*

ThP 364 **Development of Tissue Sample Preparation Method for Large-scale Quantitative Mass Spectrometry Analysis**; Yoseop Kim[1]; Hyunsoo Kim[1, 2, 3]; Minsoo Son[1]; Youngsoo Kim[2, 3, 4]; *[1]Departmet of Biomedical Engineering Seoul National University College of Engineering, jongrogu, South Korea; [2]Institute of Medical and Biological Engineering, Medical Research Center, jongrogu, South Korea; [3]Departmet of Biomedical Sciences College of Medicine, jongrogu, South Korea; [4]Departmet of Biomedical Engineering Seoul National University College of Engineering, biomedical science building 301, dahakro 101, jongro-gu, South Korea*

ThP 365 **SP2: Rapid and Automatable Contaminant Removal from Peptide Samples for Proteomic Analyses**; Michael Pereckas[1]; Matthew Waas[1]; Rachel A. Jones Lipinski[1]; Rebekah L. Gundry[1]; *[1]Medical College of Wisconsin, Milwaukee, WI*

ThP 366 **Comparing SP3, iST and S-Trap™ for Phosphopeptide Enrichment and Global Proteome Analysis**; Johannes Krumm[1]; Bernhard Kuster[2]; *[1]Chair of Proteomics and Bioanalytics, Freising, Germany; [2]Chair of Proteomics and Bioanalytics, Technical University of Munich, Freising, Germany*

ThP 367 **High-Temperature Trypsin Characterization and Comparison**; Laura K. Muehlbauer[1]; Alexander S. Hebert[2]; Joshua J. Coon[1, 2, 3, 4]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]Genome Center of Wisconsin, Madison, WI; [3]Morgridge Institute for Research, Madison, WI; [4]Department of Biomolecular Chemistry, University of Wisconsin-Madison, Madison, WI*

ThP 368 **Development of a SPE LC-MS/MS Method for the Bioanalytical Quantification of Pramlintide from Serum**; Caitlin M Dunning[1]; Mary E Lame[1]; Paula M Orens[1]; Kim Haynes[1]; Mark D Wrona[1]; *[1]Waters Corporation, Milford, MA*

ThP 369 **An Optimized In-Solution Digestion Method for Identification of Peptides from Cell Debris after Cell Lysis of RAW 264.7 Macrophage Cells**; Ada Shahinuzzaman[1]; Jayanta Kishor Chakrabarty[1]; Abu Hena Mostafa Kamal[1]; Saiful M. Chowdhury[1]; *[1]University of Texas At Arlington, Arlington, TX*

ThP 370 **An Approach for Robust Extraction and Efficient Preservation of Proteins from Urine Samples for Subsequent Quantitative Mass Spectrometry Analysis**; Xuemei Zeng[1]; Pamela S Cantrell[1]; Mai Sun[1]; Yang Liu[1]; Nathan A Yates[1,2]; *[1]Biomedical Mass Spectrometry Center, University of Pittsburgh Schools of the Health Sciences, Pittsburgh, PA; [2]Department of Cell Biology, University of Pittsburgh School of Medicine, Pittsburgh, PA*

ThP 371 **Enhanced Protonation Due to Chromium(III) during Liquid Chromatography Electrospray Ionization Mass Spectrometry**; Matthew Mireles[1]; Carolyn J. Cassady[2]; *[1]University of Alabama, Tuscaloosa, AL; [2]The University of Alabama, Tuscaloosa, AL*

ThP 372 **Automated PTMscan® Immunoaffinity Enrichment for the Capture of KGG Modified Peptides from Complex Mixtures**; Lilian Phu[1]; Shadie Nimri[2]; Anne Baldwin[3]; Nadia Martinez Martin[1]; Chris Suh[2]; Matthew P Stokes[4]; Donald S. Kirkpatrick[1]; *[1]Genentech, Inc., South San Francisco, CA; [2]PhyNexus, Inc., San Jose, Ca, CA; [3]Synthego Corporation, Redwood City, CA; [4]Cell Signaling Technology, Danvers, MA*

ThP 373 **Positive Pressure-Assisted Sample Preparation (PASP) for Proteomics**; Yang Liu[1]; Richard Lam[2]; John Laycock[2]; Nathan A Yates[1]; *[1]University of Pittsburgh School of Medicine, Pittsburgh, PA; [2]Tecan SP, Inc., Baldwin Park, CA*

ThP 374 **Immuno and Enzymatic Reactor Micro-SPE Cartridges for Rapid Protein Isolation and Digest**; Karen Duong[1]; Simin Maleknia[1]; Andrew Minett[2]; David Bishop[1]; Philip Doble[1]; *[1]University of Technology Sydney, Sydney, Australia; [2]Eprep Pty Ltd, Mulgrave, Australia*

ThP 375 **Sample Preparation for Bottom-Up Proteomics Using a Two-Stage Disposable Cartridge (ProTrap XGTM) Equipped with Chitosan-Immobilized Trypsin**; Subin R. C. K. Rajendran[1]; Alan A. Doucette[2]; *[1]Department of Chemistry, Dalhousie University, Halifax, NS; [2]Dalhousie University, Halifax, NS*

ThP 376 **Profiling the Recovery of Low Molecular Weight Proteins and Peptides Following Precipitation in the ProTrap XG**; Venus Baghalabadi; *Dalhousie University, Halifax, NS*

ThP 377 **Hands-Off: Fully Automated & TMT-Compatible Sample Preparation on the PreOn Liquid Handling Platform Employing the iST-NHS Workflow**; Fabian Hosp[1]; Doris Jansen[1]; Nils Kulak[2]; *[1]PreOmics GmbH, Planegg/ Martinsried, Germany; [2]PreOmics GmbH, Planegg/ martinsried, Germany*

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ThP 378 **Epoxidation with mCPBA: A Universal Method to Pinpoint Lipid Double-bond Positions by Tandem Mass Spectrometry**; Ting-Hao Kuo[1]; Hsin-Hsiang Chung[1]; Hsin-Yuan Chang[1]; Chiao-Wei Lin[2,3]; Ming-Yang Wang[4]; Tang-Long Shen[3]; Cheng-Chih Hsu[1]; *[1]Department of Chemistry, National Taiwan University, Taipei, Taiwan; [2]Department of Animal Science and Technology, National Taiwan University, Taipei, Taiwan; [3]Department of Plant Pathology and Microbiology, National Taiwan University, Taipei, Taiwan; [4]Department of Surgery, National Taiwan University Hospital and College of Medicine, Taipei, Taiwan*

ThP 379 **Insights into the Structural Diversity of Cardiolipins by Mathematical Modeling of LC-MS/MS Data**; Gregor Oemer[1]; Marie-Luise Edenhofer[1]; Katharina Lackner[1]; Jakob Koch[1]; Ernst R. Werner[1]; Johannes Zschocke[1]; Markus A. Keller[1]; *[1]Medical University Innsbruck, Innsbruck, Austria*

ThP 380 **Comprehensive Structural Characterization and Quantitation of Glycerophospholipids Enabled by Photochemistry and Tandem Mass Spectrometry**; Wenbo Cao[1]; Wenpeng Zhang[1,2]; Qinhua Chen[3]; Zheng Ouyang[1,2]; Xiaoxiao Ma[1]; *[1]State Key Laboratory of Precision Measurement Technology and Instruments, Department of Precision Instrument, Tsinghua University, Beijing, China; [2]Weldon School of Biomedical Engineering and Department of Chemistry, Purdue University, West Lafayette, IN 47906; [3]Affiliated Dongfeng Hospital, Hubei University of Medicine, Shiyan, China*

ThP 381 **Lipid Omega Analyzer- Lipidomic Data Analysis System with C=C Location Identification Capability**; Donghui Zhang[1]; Wenpeng Zhang[2,3]; Zheng Ouyang[1]; Yu Xia[2]; *[1]State Key Laboratory of Precision Measurement Technology and Instrument, Department of Precision Instruments, Tsinghua University, Beijing, China; [2]Department of Chemistry, Tsinghua University, Beijing, China; [3]Department of Chemistry Purdue University, West Lafayette, IN*

ThP 382 **An LC-PB-MS/MS Workflow for Characterizing Phosphatidylinositols and Phosphatidylglycerols with Double Bond Location**; Tian Xia[1]; Wenpeng Zhang[1,2]; Hanlin Ren[1]; Yu Xia[1]; *[1]Department of Chemistry, Tsinghua University, Beijing, China; [2]Department of Chemistry, Purdue University, West Lafayette, IN*

ThP 383 **Locating C=C Bonds in Unsaturated Lipids *via* *Visible-Light Paternò–Büchi Reaction***; Hai-Fang Li[1]; Xiaoxiao Ma[1]; Yu Xia[1]; Zheng Ouyang[1]; *[1]Tsinghua University, Beijing, China*

ThP 384 **UHPLC-IMS-MS as a New Tool for the Characterization of the Membrane Lipids of *Pseudomonas aeruginosa.***; Estelle Deschamps[1,2]; Isabelle Schmitz-Afonso[1]; Annick Schaumann[2]; Corinne Loutelier-Bourhis[1]; Stéphane Alexandre[2]; Emanuelle Dé[2]; Carlos Afonso[1]; *[1]Laboratoire COBRA, UMR6014, University of Rouen, Mont-Saint-Aignan, France; [2]Laboratoire PBS, UMR6270, University of Rouen, Mont-Saint-Aignan, France*

ThP 385 **Localizing Carbon-Carbon Double Bond Position of Unsaturated Lipid Isomers by m-CPBA Epoxidation and ESI/MALDI Mass Spectrometry**; Yu Feng[1]; Bingming Chen[1]; Qinying Yu[1]; Meng Xu[2]; Lingjun Li[1,2]; *[1]School of Pharmacy, University of Wisconsin, Madison, WI; [2]Department of Chemistry, University of Wisconsin, Madison, WI*

ThP 386 **MS Determination of Double Bond Position of Lipids at Single-Cell Level**; Yanlin Zhu[1]; Zhibo Yang[1]; *[1]University of Oklahoma, Norman, OK*

ThP 387 **Localization of Cyclopropane Modifications in Bacterial Lipids *via* Ultraviolet Photodissociation Mass Spectrometry**; Molly S Blevins[1]; Jennifer S Brodbelt[1]; M. Stephen Trent[2]; *[1]University of Texas at Austin, Austin, TX; [2]University of Georgia, Athens, GA*

ThP 388 **Widely Targeted Lipidomics Profiling (WTLP) with Unit Dalton Resolution Using the Sciex 6500+ QTRAP**; Yunping Qiu[1]; Mackenzie J J Pearson[2]; Min Cai[1]; Cyrus Papan[3]; Irwin J Kurland[4]; *[1]Albert Einstein College of Medicine, Bronx, NY; [2]Sciex, Framingham, MA; [3]SCIEX, Darmstadt, Germany; [4]Albert Einstein CollegeMed, Bronx, NY*

ThP 389 **Sphingolipid Metabolism as a Molecular Marker of Cellular Dysfunction in Drug-Induced Liver Injury**; Linhao Li[1]; Mohammad I Ansari[1]; Hongbing Wang[1]; Jace W Jones[1]; *[1]University of Maryland, School of Pharmacy, Baltimore, MD*

ThP 390 **Enhancing Shotgun Lipidomics by Structural Characterization of Cardiolipins *via* Ultraviolet Photodissociation (UVPD)**; Luis A Macias[1]; Clara L. Feider[1]; Livia S Eberlin[1]; Jennifer S Brodbelt[1]; *[1]University of Texas - Austin, Austin, TX*

ThP 391 **Improved Lipid Annotation Depth Using Automatically Generated Inclusion and Exclusion Lists on an Orbitrap-Based Mass Spectrometer**; Sven Hackbusch[1];

David Peake[1]; Reiko Kiyonami[1]; [1]*Thermo Fisher Scientific, San Jose, CA*

ThP 392 **High-Throughput Analysis of Glycerol Lipids with C=C Localization *via* RPLC-PB-MS/MS**; Elissia Franklin[1]; Yu Xia[2]; [1]*Purdue University, West Lafayette, IN;* [2]*Tsinghua University, Beijing, China*

ThP 393 **Evaluation of Surface Induced Dissociation in Conjunction with Ion Mobility-Mass Spectrometry for Lipid Structural Characterization**; Rachel A. Harris[1]; Jody C. May[1]; Sophie R. Harvey[2]; Vicki Wysocki[2]; John A. McLean[1]; [1]*Vanderbilt University, Nashville, TN;* [2]*The Ohio State University, Columbus, OH*

ThP 394 **Untargeted Macrolipidomic Profiling of Plant-Based Oils**; Juan Aristizabal-Henao[1]; Ningombam Sanjib Meitei[2]; Ken D. Stark[1]; [1]*University of Waterloo, Waterloo, ON;* [2]*PREMIER Biosoft, Palo Alto, CA*

ThP 395 **Higher Confidence Annotations of Target Lipids Enabled by Trapped Ion Mobility MS in Combination with Machine Learning Based CCS Prediction**; Matthias Szesny[1]; Sebastian Wehner[1]; Heiko Neuweger[1]; Ulrike Schweiger-Hufnagel[1]; Sven W. Meyer[1]; Aiko Barsch[1]; Nikolas Kessler[1]; Lucy Woods[1]; [1]*Bruker Daltonics, Bremen, Germany*

ThP 396 **Ceramide Analysis on a MALDI-TOF Platform: Matrix, Adduct, and Fragmentation Optimization**; Anh Tran[1]; Jace W Jones[1]; [1]*University of Maryland, School of Pharmacy, Department of Pharmaceutical Sciences, Baltimore, MD*

ThP 397 **A Novel Data Strategy Towards an Integrated LC/MS- 1H NMR Workflow for Identifying Unknown Lipids**; Jiajun Lei[1]; Rohit Mahar[1]; Ram Khattri[1]; Matthew E. Merritt[1]; Timothy J. Garrett[1]; Richard A Yost[1]; [1]*University of Florida, Gainesville, FL*

ThP 398 **Leveraging Multidimensional Separations to Enhance Traditional LC-MS Lipidomics Workflows**; Sarah M. Stow[1]; Mark Sartain[2]; Aivett Bilbao[3]; Bryson C. Gibbons[3]; Juli Salcedo[2]; Xiangdong Li[2]; Adithya Murali[2]; Jeremy Koelmel[4]; Robin H.J Kemperman[4]; John C. Fjeldsted[2]; [1]*Agilent Technologies, Santa Clara, CA;* [2]*Agilent Technologies, Inc., Santa Clara, CA;* [3]*Pacific Northwest National Laboratory, Richland, WA;* [4]*University of Florida, Gainesville, FL*

ThP 399 **Dual Derivatization Strategy for the LCMS Analysis of Plasmenyl Glycerophospholipids**; Samuel W Shields[1]; Carlos R Canez[1]; Peter J Pallister[1]; Jeffrey M Manthorpe[1]; Jeffrey C Smith[1]; [1]*Carleton University, Ottawa, ON*

ThP 400 **Oxygen Attachment Dissociation MS/MS for Differentiation between Cis and Trans Fatty Acids**; Hidenori Takahashi[1]; Yuji Shimabukuro[2]; Daiki Asakawa[3]; Shosei Yamauchi[4]; Shinichi Iwamoto[4]; Motoi Wada[2]; Koichi Tanaka[4]; [1]*Shimadzu Corporation, Kyoto, Japan;* [2]*Doshisha University, Kyoto, Japan;* [3]*AIST, Tsukuba, Japan;* [4]*Shimadzu corp., Kyoto, Japan*

ThP 401 **Establishment of a Novel Identification Algorithm for Non-Targeted LCMS Workflows Using a New and Effective Deconvolution Technique**; Yasuto Yokoi[1]; Takefumi Moriya[1]; Takao Nakajima[1]; David A. Peake[2]; Reiko Kiyonami[3]; [1]*Mitsui Knowledge Industry Co., Ltd., Tokyo, Japan;* [2]*Thermo Fisher Scientific, Sunnyvale, CA;* [3]*Thermo Fisher Scientific, Sunnyvale, CA*

ThP 402 **Structural Identification of Phosphatidylcholine Isomers Directly from Mouse Brain Tissue Using Electron Induced Dissociation on an FT-ICR Mass Spectrometer**; Matthias-Erich N Born[1]; Boone M. Prentice[1]; [1]*University of Florida, Gainesville, FL*

ThP 403 **Global Measurement of Mouse Brain Lipids**; Russell Louis Denton[1]; Kyle J Cutler[2]; Conner Holman[2]; Joseph Creery[2]; John C Price[2]; [1]*Brigham Young University, Provo, UT;* [2]*Brigham Young University, Provo, Utah*

ThP 404 **Lipidomics Analysis in Niemann-Pick C Cells**; Jonathan Paz; *EPFL, Lausanne, Switzerland*

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ThP 405 **Mass Spectrometry Methods for Bacterial Infection Diagnosis**; Yingdi Zhu[1]; Hubert H. Girault[1]; [1]*Ecole Polytechnique Fédérale de Lausanne (EPFL), Sion, Switzerland*

ThP 406 **Studying Non-Covalent Interactions between G Protein-Coupled Receptors and miniGα Proteins by MALDI Mass Spectroscopy**; Na Wu; *ETHz, zurich, Switzerland*

ThP 407 **Detecting Protein-Peptide Interactions Utilizing SAMDI and MALDI-TOF**; Hilda Hernandez-Barry[1]; Gary Wilson[1]; Erica Vanderporten[1]; Yue Fu[1]; Maciej Paluch[1]; Phil Hass[1]; Rami Hannoush[1]; Yichin Liu[1]; Kelly Loyet[1]; [1]*Genentech, South San Francisco, CA*

ThP 408 **Direct Identification of Phytoplankton Pigments in Sea Water Samples Using Electron Transfer MALDI MS**; Luis Miguel Díaz[1]; Marianny Y. Combariza[1]; Cristian Blanco-Tirado[1]; Juan Ramirez[1]; Mayra C. Morales[2]; Maria I. Criales[1]; Andres Franco Herrera[2]; [1]*Universidad Industrial de Santander, Bucaramanga, Colombia;* [2]*Universidad Jorge Tadeo Lozano, Santa Marta, Colombia*

ThP 409 **MSn Analyses for Tryptophan-Conjugated ADC Mimic by Miniature MALDI Digital Ion Trap Mass Spectrometer (MALDI-DIT-MS)**; Hideharu Shichi[1]; Shuichi Nakaya[1]; Katsuya Maruyama[2]; Kosuke Hosoi[1]; Takashi Nishikaze[1]; Koichi Kojima[1]; Kei Kodera[1]; Sadanori Sekiya[1]; Shinichi Iwamoto[1]; Kounosuke Oisaki[2]; Motomu Kanai[2]; Koichi Tanaka[1]; [1]*SHIMADZU, Kyoto, Japan;* [2]*Graduate School of Pharmaceutical Sciences, The University of Tokyo, Bunkyo, Japan*

ThP 410 **A High-Throughput Multiplexed Assay Platform for Monitoring Protein Abundance in 96-Well Cell Cultures or Product Profiles from Enzyme-Substrate Reactions**; Sergey Mamaev[1]; Jeffrey C. Silva[1]; Camilla Worsfold[1]; Vladislav B. Bergo[1]; [1]*ADEPTRIX CORP., Beverly, MA*

ThP 411 **Development of a Quantitative Peptide MALDI MS Method for Indirect Determination of Amine Density of an Amine Surface**; Jason M Peterson[1]; Loren J Howell[1]; James G Boyd[1]; Gaurav Saini[1]; Patrick Walsh[1]; Olgica Trenchevska[1]; [1]*HealthTell Inc, Chandler, AZ*

ThP 412 **Characterization of Peptide "Primordial Soups" using MALDI-TOF and MALDI-FTICR MS**; Jabbarrius N. Ervin[1]; Marcos Bouza Areces[2]; Facundo M. Fernandez[2]; Jay G. Forsythe[1]; [1]*College of Charleston, Charleston, SC;* [2]*Georgia Institute of Technology, Atlanta, GA*

ThP 413 **MALDI-directed Region Selection for Laser Ablation Tissue Microsampling**; Kelin Wang[1]; Fabrizio Donnarumma[1]; Michael Pettit[2]; Touradj Solouki[2]; Kermit K. Murray[1]; [1]*Louisiana State University, Baton Rouge, LA;* [2]*Baylor University, Waco, TX*

ThP 414 **Plasmonic Nanoshells for Drug, Metabolite and Bacteria Detection with Mass Spectrometry**; Lin Huang[1]; Kun Qian[2]; [1]*Shanghai Jiao Tong University, Shanghai, China;* [2]*Shanghai Jiao Tong University, Shanghai, China*

ThP 415 **Comparison of Diethyl Dithiocarbamate and Pyrrolidine Dithiocarbamate for Cisplatin and Copper Chelation by MALDI-TOF**; Yi-Feng Dai[1]; Hung-Wei Yang[2]; Chiung-Yin Huang[3]; Kuo-Chen Wei[3]; Hay-Yan J. Wang[4,5]; [1]*National Sun Yat-sen University, Kaohsiung, Taiwan;* [2]*Institute of Medical Science and Technology, National Sun Yat-sen University, Kaohsiung, Taiwan;* [3]*Chang Gung Memorial Hospital, Tainan, Taiwan;* [4]*Department of Biological Sciences, National Sun Yat-sen University, Kaohsiung, Taiwan;* [5]*Doctoral Degree Program in Marine Biotechnology, National Sun Yat-sen University and Academia Sinica, Kaohsiung, Taiwan*

ThP 416 **High-Throughput MALDI-TOF Stem Cell Quality Assurance**; Stephen Zambrzycki[1]; Gilad Doron[2]; Johnna S Temenoff[2]; Facundo M Fernandez[1]; [1]*Georgia Institute of Technology, School of Chemistry and Biochemistry, Atlanta,*

Georgia; [2]Georgia Institute of Technology, Department of Biomedical Engineering, Atlanta, Georgia

ThP 417 **AP-MALDI-Q-IMS-TOF MS as a Highly Accurate MS Profiling Platform for Speciation/Biotyping**; Cristian Piras[1]; Oliver J Hale[1]; Barney Jones[1]; Nick Taylor[1]; Mike Morris[2]; Christopher K Reynolds[1]; Rainer Cramer[1]; *[1]University of Reading, Reading, United Kingdom; [2]Waters Corporation, Wilmslow, United Kingdom*

MALDI: FUNDAMENTALS AND INSTRUMENTATION
418-421

ThP 418 **Insights on Cation-Adduct Formation in MALDI Mass Spectrometry**; Jonas B Metternich[1]; Martin F Czar[1]; Mario F Mirabelli[1]; Giovanni L Bartolomeo[1]; Renato Zenobi[1]; *[1]ETH Zurich, Zurich, Switzerland*

ThP 419 **Enhanced Protonation upon Addition of Chromium(III) During Matrix-Assisted Laser Desorption Ionization**; Nnenna E Dieke[1]; Carolyn J Cassady[1]; *[1]The University of Alabama, Tuscaloosa, AL*

ThP 420 **Ion Source Cleaning Plate for Clinical MALDI-TOF System**; Heesung Kang[1]; Joo Yeon Oh[1]; Yang Sun Kim[1]; *[1]ASTA, Suwon-si, South Korea*

ThP 421 **Utilizing a Cold-Mist Nebulizer to Perform Matrix Deposition in MALDI MS Analyses of Complex Samples and Tissue Slices**; Eugene Moskovets[1]; Vladimir M. Doroshenko[1]; Alexey Gapeev[2]; Shelley N. Jackson[3]; Ludovic Muller[3]; Amina S. Woods[3]; *[1]MassTech Inc, Columbia, MD; [2]Millis Scientific Inc, Baltimore, MD; [3]NIH/ NIDA-IRP, Baltimore, MD*

MALDI: SAMPLE PREPARATION
422-430

ThP 422 **On-Target Recrystallization of 2,5-Dihydroxybenzoic Acid Using Acetonitrile Droplet as an Enhancement of Surface Homogeneity for MALDI-MS Dried-Droplet Sample Preparation**; Huu-Quang Nguyen[1]; Dabin Lee[1]; Yeoseon Kim[1]; Min Sun Kim[2]; Kyoung-Soon Jang[3]; Jeongkwon Kim[1]; *[1]Chungnam National University, Daejeon, South Korea; [2]Scientific Instruments Reliability Assessment Center, Korea Basic Science Institute, Daejeon, South Korea; [3]Biomedical Omics Center, Korea Basic Science Institute, Daejeon, South Korea*

ThP 423 **High-Speed Characterization of Candle Waxes Using Surface-Assisted Laser Desorption/Ionization Mass Spectrometry (SALDI-MS) with Etched Silver Foil as Substrates**; Andreas Schnapp[1]; Ann-Christin Niehoff[1]; *[1]Shimadzu Europa GmbH, Duisburg, Germany*

ThP 424 **Nanodiamond Assisted MALDI-MS Analysis of High Mass Proteins in the Nanomolar Concentration Range**; Avinash Adhikrao Patil[1]; Mhikee Janella N. Descanzo[1]; Chen-Hao Wen[1]; Wen-Ping Peng[1]; *[1]National Dong Hwa University, Shoufeng, Taiwan*

ThP 425 **Serial Detachment of Amino Acids from Microwave-Assisted Weak Acid Protein Hydrolysis**; Jihyun Paek[1]; Jeongkwon Kim[1]; *[1]Chungnam National University, Daejeon, South Korea*

ThP 426 **Assessing the Effects of Tissue Fixation, Freezing, Embedding, and Washing on the Global Lipidome Utilizing MALDI FT-ICR IMS**; Marissa A. Jones[1,2]; Jeffrey M. Spraggins[1,2,3]; Nathan Heath Patterson[1,4]; William J. Perry[1,2]; Richard M. Caprioli[1,2,4,5,6]; *[1]Mass Spectrometry Research Center, Vanderbilt University, Nashville, TN; [2]Department of Chemistry, Vanderbilt University, Nashville, TN; [3]Department of Biochemistry, Vanderbilt University, Nashville, Tennessee; [4]Department of Biochemistry, Vanderbilt University, Nashville, TN; [5]Department of Pharmacology, Vanderbilt University, Nashville, TN; [6]Department of Medicine, Vanderbilt University, Nashville, TN*

ThP 427 **N-glycan MALDI Fingerprinting and All-In-One Reducing-End Derivation Matrix Optimization**; Nicolas Eskenazi[1]; Ophelia Djimatey[1]; Chiara Giangrande[1]; Joëlle Vinh[1]; *[1]SMBP, ESPCI, PSL University, PARIS, France*

ThP 428 **Simple Surface Modification for Enhancing Carbohydrate Ion Sensitivity in Matrix-Assisted Laser Desorption/Ionization Time-Of-Flight Mass Spectrometry**; Chia-Hsin Chi[1]; Yu-Meng Ou[1,2]; Yi-Sheng Wang[1]; *[1]Genomics Research Center, Academia Sinica, Taipei, Taiwan; [2]Department of Chemistry, National Taiwan University, Taipei, Taiwan*

ThP 429 **Toward Seamless Incorporation of Paternò–Büchi Carbon-Carbon Double Bond Localization in Common MALDI-MSI Workflow**; Andrew E Paulson[1]; Young-Jin Lee[1]; *[1]Iowa State University, Ames, IA*

ThP 430 **Rapid Isolation of Peptides and Proteins from Biological Fluids for Proteomic Analysis by MALDI-TOF Mass Spectrometry**; Ryan Walsh[1]; Matt Texter[2]; Robert English[3]; Eric Weaver[4]; *[1]Shimadzu Scientific Instruments Corp., Columbia, MD; [2]Shimadzu Scientific Instruments, Inc, Columbia, MD; [3]Shimadzu Scientific Instruments, Inc., Columbia, Maryland; [4]University of Texas, Arlington, Arlington, TX*

METABOLOMICS: CLINICAL APPLICATIONS
431-449

ThP 431 **Utilizing Microfluidic Devices to Evaluate Cellular Metabolism of Therapeutics with Online Mass Spectrometric Detection**; Campbell B Mousseau[1]; Chengpeng Chen[2]; R. Scott Martin[2]; Amanda B. Hummon[1]; *[1]The Ohio State University, Columbus, OH; [2]Saint Louis University, St. Louis, MO*

ThP 432 **Integrated Workflow with Quality Control for Large Cohort and Clinical Metabolomics Research Using Robust Hardware and Signal Correction**; Sebastian Goetz[1]; Ulrike Schweiger-Hufnagel[1]; Matthias Szesny[1]; Aiko Barsch[1]; Sven W. Meyer[1]; Matthew R. Lewis[2]; Nikolas Kessler[1]; *[1]Bruker Daltonics, Bremen, Germany; [2]Imperial College London, London, United Kingdom*

ThP 433 **Dynamic Assessment of the Human Saliva Structural Lipidome using MS/MSALL Shotgun Lipidomics for Population Health Applications**; Valerie Bussberg[1]; Hannah Rockwell[1]; Gramoz Kondakci[1]; Emily Y. Chen[1]; Fei Gao[1]; Niven R. Narain[1]; Michael A. Kiebish[1]; *[1]BERG, LLC, Framingham, MA*

ThP 434 **Development of a Functional Neurometabolomics Platform to Enable MOA and Functional Studies in Drug Development and Precision Medicine**; Bennett Greenwood[1]; Collin Hill[1]; Vladimir Tolstikov[1]; Reinhard Roessler[1]; Christine Denny[2]; Josephine McGowan[2]; Vivek Vishnudas[1]; Rangaprasad Sarangarajan[1]; Niven R. Narain[1]; Michael A. Kiebish[1]; *[1]BERG, LLC, Framingham, MA; [2]Columbia University, New York, NY*

ThP 435 **Metabolomics Analysis of Adults-Onset Still's Disease by SWATH-MS**; Chien-Chen Lai[1]; Hsuan-Jen Chen[1]; *[1]National Chung Hsing University, Taichung, Taiwan*

ThP 436 **Influenza Viral Infection Detection in Seconds Using LDTD-MS and Machine Learning**; Pier-Luc Plante[1,2]; Élina Francovic-Fontaine[1,2]; Francis Brière[1,2]; Nancy Boucher[2]; Julie Carbonneau[2]; Marie-Ève Hamelin[2]; Guy Boivin[2]; Jacques Corbeil[1,2]; *[1]Université Laval, Quebec, Quebec; [2]Infectiology Research Centre, CHU de Québec, Laval University, Québec, QC*

ThP 437 **Multiomics Analysis of The Metabolome and Intestinal Microbiome of Antibiotics versus Pathogen-Specific Monoclonal Antibodies**; Omari Jones-Nelson[1]; Matthew Glover[1]; Andrey Tovchigrechko[1]; Taylor Cohen[1]; Fiona Fernandes[2]; Udaya Rangaswamy[2]; Liu Hui[2]; David Tabor[2]; Paul Warrener[1]; Jose Martinez[1]; Wen Yu[1]; Gina Dangelo[1]; Sonja Hess[3]; Bret Sellman[1]; *[1]MedImmune, Gaithersburg,*

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MD; [2]MedImmune, South San Francisco, California; [3]MedImmune, Gaithersburg

ThP 438 **A Novel Derivatization LC-MS/MS-Based Method for Quantifying Metanephrines from Dried Blood Spots for the Diagnosis of Pheochromocytomas and Paragangliomas (PPCs/PPGLs)**; Vincent R. Richard[1]; Rene Zahedi[1]; Shaun Eintracht[2]; Christoph H. Borchers[1,3,4,5]; *[1]Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC; [2]Department of Diagnostic Medicine, Jewish General Hospital, McGill University, Montreal, QC; [3]University of Victoria-Genome BC Proteomics Centre, Victoria, BC; [4]Department of Biochemistry and Microbiology, University of Victoria, Victoria, BC; [5]Gerald Bronfman Department of Oncology, Jewish General Hospital, McGill University, Montreal, QC*

ThP 439 **High Resolution Mass Spectrometry Newborn Screening Applications for Quantitative Analysis of Amino Acids and Acylcarnitines from Dried Blood Spots**; C. Austin A Pickens[1]; Konstantinos Petritis[1]; *[1]Centers for Disease Control and Prevention, Chamblee, GA*

ThP 440 **Development of a New Vitamin D Assay and Its Application to Profile Vitamin D Metabolites in a Pediatric Population**; Brian C DeFelice[1]; Theresa L Pedersen[1]; Hanan Shorrosh[2]; Randi K. Johnson[2]; Jennifer A Seifert[2]; Jill M. Norris[2]; Oliver Fiehn[3]; *[1]University of California, Davis, Davis, CA; [2]University of Colorado, Denver - Anschutz, Aurora, CO; [3]University of California Davis, Davis, CA*

ThP 441 **Metabolomic Studies in Newborn Exposed to Zika Virus**; Danielle Zildeana Souza Furtado[1]; Luiz André Zanluqui[1]; Cleber N. Barretos[1]; Fabiana A. Marques[2]; Regina V Oliveira[3]; Nilson Antonio Assuncao[1]; *[1]Universidade Federal de São Paulo (UNIFESP), São Paulo, Brazil; [2]Instituto Federal de Educação, Ciência e Tecnologia Goiano, Campus Ceres., Ceres, Brazil; [3]Universidade Federal de São Carlos, São Carlos, Brazil*

ThP 442 **New Secondary Electrospray Ionization Configuration with Improved Background Levels and Repeatability for Online Analysis of Relevant Metabolites in Breath**; Pedro A. Barreiro[1]; Miriam Macia[1]; Kapil D. Singh[2]; Pablo Sinues[2]; Guillermo Vidal-De-Miguel[1]; *[1]Fossil Ion Technology, Madrid, Spain; [2]University of Basel, Basel, Switzerland*

ThP 443 **Metabolic Profile of Saliva and Biofilm of 30 Patients during Hospitalization in ICU**; Monira Samaan Kallas Kallas[1]; Meriellen Dias[2]; Isaac Castro[1]; Maria Anita Mendes[2]; Luciano Cesar Pontes Azevedo[1]; *[1]Sirio Libanes Hospital,, São Paulo, Brazil; [2]Dempster MS Lab- Poli-USP, Sao Paulo, Brazil*

ThP 444 **Metabolic Assessment of Multi-Risk Factors of Alzheimer's Disease Based on Integrative Metabolomic Analysis**; Soo Jin Park[1]; Eosu Kim[2]; Soo ah Jang[2]; Do Yup Lee[1]; *[1]kookmin university, Seoul, South Korea; [2]Yonsei University College of Medicine, Seoul, South Korea*

ThP 445 **MALDI-FTMS and NMR Serum Analysis for Biomarker Based Determination of Diabetes During Pregnancy**; Franklin E. Leach Iii[1]; Jacquelyn Walejko[1]; Maureen Keller-Wood[2]; Arthur S. Edison[1]; *[1]University of Georgia, Athens, GA; [2]University of Florida, Gainesville, FL*

ThP 446 **Biomarker Discovery and Validation for Delirium Syndrome Using Mass Spectrometry-Based Metabolomics Analysis of Serum Samples**; Don E. Davis, Jr.[1,2,3,4]; Simona G. Codreanu[1,2,3,4]; Stacy D. Sherrod[1,2,3,4]; Jennifer Colby[5]; Jin H. Han[6]; John A. McLean[1,2,3,4]; *[1]Vanderbilt University Department of Chemistry, Nashville, TN; [2]Vanderbilt Institute of Chemical Biology, Nashville, TN; [3]Center for Innovative Technology, Nashville, TN; [4]Vanderbilt Institute for Integrative Biosystems Research and Education, Nashville, TN; [5]Vanderbilt University Medical Center Department of Pathology, Microbiology and Immunology, Nashville, TN; [6]Vanderbilt University Medical Center Department of Emergency Medicine, Nashville, TN*

ThP 447 **Metabolic Preference Assay for Rapid Diagnosis of Bloodstream Infections**; Thomas Rydzak[1]; Ryan A Groves[1]; Heather Semeniuk[2]; Rajnigandha Pushpker[1]; Ruichuan Zhang[1]; Daniel Gregson[2]; Deirdre Church[2]; Ian A Lewis[1]; *[1]University of Calgary, Calgary, AB; [2]Calgary Laboratory Services, Alberta Health Services, Calgary, AB*

ThP 448 **Investigating the Complex Interaction between Host Prostate Cancer Cells and Common Microbes Using LC-IM-QTOF-MS Based Platform**; Sumankalai Ramachandran[1]; Minas Sakellakis[1]; Gary Gallick[1]; Christopher Logothetis[1,2]; Mark Titus[1]; *[1]Department of Genitourinary Medical Oncology, The University of Texas MD Anderson Cancer Center, Houston, TX, Houston, TX; [2]Department of Clinical Therapeutics, University of Athens, Athens, Greece*

ThP 449 **UPLC-MS Based Plasma Metabolomics Reveal Aromatic Amino Acids Metabolites are Associated with Nonalcoholic Steatohepatitis**; Nisreen Nimer[1,2]; Zeneng Wang[2]; Ina Nemet[2]; Valentin Gogonea[1,2]; Stanley L Hazen[1,2]; *[1]Cleveland State University, Cleveland, OH; [2]Cleveland Clinic, Cleveland, OH*

METABOLOMICS: GENERAL II
450-478

ThP 450 **Novel Metabolite Interactions between Branched Amino Acid Aminotransferase 2 (BCAT2), Phenyl Compounds, and Biocytin**; Carol Nilsson[1]; Kevin G. Hicks[2]; Jared Rutter[2]; *[1]Lund University, Lund, Sweden; [2]University of Utah School of Medicine, Salt Lake City, UT*

ThP 451 **Metabolomics Analysis of IL-2 and IL-15 Expanded γ9δ2 T Cells Co-Cultivated with Cancer Cell Lines**; Thomas P. Wyche[1]; Rurun Wang[1]; Kalyn Schriefer[1]; Samantha O'Hara[1]; Jason Killough[1]; Dario Gutierrez[1]; Theodore Sana[1]; *[1]Merck & Co., Inc., Cambridge, MA*

ThP 452 **Where Does Tcruzi Hide? A Mass Spectrometric Study of *T. cruzi* Infection in Mouse Models.**; Ekram Hossain[1]; Sharon Lostracco-Johnson[2]; Diane Thomas[2]; Laura-Isobel McCall[1]; *[1]University of Oklahoma, Norman, OK; [2]UCSD, San Diego, CA*

ThP 453 **Development of Chemical Isotope Labeling Nanoflow LC-MS for Profiling Hydroxyl Submetabolome of Small Numbers of Cells**; Xian Luo[1]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB*

ThP 454 **Rapid Quantification of Extremely Polar Metabolites in Biological Fluids Using Negative Electrospray HILIC-Mass Spectrometry**; Xiaoding Wang[1]; Lianggiao Bian[2]; Maciej Kukula[2]; Zhao Wang[1]; *[1]Division of Cardiology, Department of Internal Medicine, University of Texas Southwestern Medical Center, Dallas, Texas; [2]Shimadzu Center for Advanced Analytical Chemistry, University of Texas at Arlington, Arlington, TX*

ThP 455 **Metabolomic Profiling Shows that Glutathione Depletion Is Rescued Along with Growth Rate in Yeast Methionine Auxotrophs**; Matthew A. Kukurugya[1]; Bernd J. Wranik[1]; Tina Mahatdejkul-Meadows[1]; R. Scott McIsaac[1]; Bryson D. Bennett[1]; *[1]Calico Life Sciences, South San Francisco, CA*

ThP 456 **Analysis of Single Liver Cells to Study Drug Uptake, Metabolism and Effects on Endogenous Metabolome at the Single Cell Level**; Liliana Pedro[1]; Patrick Rudewicz[1]; *[1]Novartis Institutes for Biomedical Research, Emeryville, CA*

ThP 457 **Evaluation of Inter-protocol Quality Control Samples Used for Metabolomic Analyses**; Bethanne M. Warrack[1]; Michael D. Reily[1]; Petia Shipkova[1]; Joelle Onorato[1]; *[1]Bristol-Myers Squibb, Princeton, NJ*

ThP 458 **Development and Validation of a High Throughput Metal Ion Panel of 23 Elements for Analysis of Bio Fluids**; Matthew T Doyle[1]; Richard Robinson[1]; Afton Starling[1]; Brent Overcash[1]; Lori Wright[1]; Fred Hubbard[1]; Anne Evans[1]; Luke Miller[1]; *[1]Metabolon, Inc., Durham, NC*

ThP 459 **Modelling Cancer Lipogenesis Using LA-REIMS Metabolic Flux analysis in Breast Cancer Cell Lines**; Seyma Turkseven[1]; Nikolaos Koundouros[2]; Simon Cameron[3]; Alvaro Perdones-Montero[3]; Renata Soares[3]; Luisa Doria[3]; George Poulogiannis[2]; Zoltan Takats[3]; *[1]Imperial College London, London, United Kingdom; [2]Institute of Cancer Research, London, United Kingdom; [3]Imperial College, London, United Kingdom*

ThP 460 **Ion-Pair Selection Method for Pseudotargeted Metabolomics Based on SWATH MS Acquisition and Its Application in Type 2 Diabetes study**; Xinjie Zhao[1,2]; Lichao wang[1,2]; Benzhe Su[3]; Zhongda Zeng[1]; Chao Li[3]; Wangjie Lv[1,2]; Qiuhui Xuan[1,2]; Lina Zhou[1,2]; Xin Lu[1,2]; Xiaohui Lin[1,2]; Guowang Xu[1,2]; *[1]CAS Key Laboratory of Separation Science for Analytical Chemistry, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, China; [2]University of Chinese Academy of Sciences, Beijing, China; [3]School of Computer Science & Technology, Dalian University of Technology, Dalian, China*

ThP 461 **A Comprehensive Heart Metabolome Enabled by Ultra-High Resolution Fourier-Transform Ion Cyclotron Resonance Mass Spectrometry (FTICR-MS)**; Benjamin Wancewicz[1]; Yutong Jin[1]; Yanlong Zhu[1]; Ying Ge[1]; *[1]UW Madison, Madison, WI*

ThP 462 **Large-Scale Metabolomic Analysis of Hydrophilic Metabolites Using Hydrophilic Interaction Liquid Chromatography Tandem Mass Spectrometry with a Novel Polymer-Based Amino Column**; Kohta Nakatani[1]; Yoshihiro Izumi[1]; Masatomo Takahashi[1]; Keita Sakurai[2]; Michio Butsugan[2]; Takeshi Bamba[1]; *[1]Medical Institute of Bioregulation, Kyushu University, Fukuoka, Japan; [2]Hitachi Chemical Techno Service Co., Ltd., Ibaraki, Japan*

ThP 463 **Identification of a Malate-Aspartate Shuttle Mediated Mechanism Supporting Drug Resistance in Lung Cancer Cells Triggered by Reduced GLUL Expression**; Anders Nordstrom[1]; Magesh Muthu[1]; *[1]Umea University, Umeå, Sweden*

ThP 464 **Next Generation Metabolomics Approach for Isolation and Higher Throughput Annotations of Metabolites from *Medicago truncatula* Using UHPLC-MS2-SPE-NMR**; Anil Bhatia[1,2]; Feng Qiu[1,3]; Dennis Fine[4]; Daniel Wherritt[4,5]; Zhentian Lei[1,2]; Lloyd W. Sumner[1,2]; *[1]Biochemistry Department, University of Missouri, Columbia, MO; [2]MU Metabolomics Center, University of Missouri, Columbia, MO; [3]International Flavors & Fragrances, Union Beach, NJ; [4]The Samuel Roberts Noble Foundation, Ardmore, OK; [5]University of Texas at San Antonio, San Antonio, TX*

ThP 465 **Mass Spectrometric Analysis of Metabolic Profile Alterations in Cataractous Lenses Due to Point Mutations in Two Alpha Crystallins**; Cheryl Frankfater[1]; Stephanie Bozeman[2]; Paul Hamilton[2]; Fong-Fu Hsu[1]; Usha Andley[2]; *[1]NIH/NIGMS Biomedical Mass Spectrometry Resource, Washington University School of Medicine, St. Louis, MO; [2]Department of Ophthalmology and Visual Sciences, Washington University School of Medicine, St. Louis, MO*

ThP 466 **Untargeted and Targeted Metabolomics Approach for Characterizing the Hypoxia-Induced Metabolomic Alterations in Primary and Metastatic Colorectal Cancer**; Sujatha Chilakala[1]; Colin Flinders[1]; Ah Young Yoon[1]; Mario M Alba[1]; Shannon M Mumenthaler[1]; Jonathan E Katz[1]; *[1]Lawrence J. Ellison Institute for Transformative Medicine of USC, Los Angeles, CA*

ThP 467 **Quatitalon of Glycine Using LC-MS to Investigate Its Role in Sex-Specific Association with Coronary Heart Diseases *in vivo* Studies**; Ah Young Yoon[1]; Nicholas C. Woodward[2]; Janet Gukasyan[2]; Sujatha Chilakala[1]; Hooman Allayee[2]; Jonathan E Katz[1]; *[1]Lawrence J. Ellison Institute for Transformative Medicine of USC, Los Angeles, California; [2]University of Southern California, Los Angeles, California*

ThP 468 **Integrating LC/MS-Based Metabolomics and Solid-State NMR for Total Accounting of Carbon**; Miriam Sindelar[1,2]; Xiangfeng Niu[1,2]; Jacob Schaefer[1]; Brian N Finck[2]; Gary J Patti[1,2]; *[1]Washington University in St. Louis, St. Louis; [2]Washington University School of Medicine in St. Louis, St. Louis, MO*

ThP 469 **Metabolic Phylogeny: Evidence for Speciation through Metabolic Selection in the Evolution of Borrelia, the Causative Agent of Lyme Disease**; Ryan A Groves[1]; Thomas Rydzak[1]; Mildred Castellanos[2]; Peter Kraiczy[3]; George Chaconas[2]; Ian A Lewis[1]; *[1]Lewis Research Group, Department of Biological Sciences, University of Calgary, Calgary, AB; [2]Department of Biochemistry and Molecular Biology, University of Calgary, Calgary, AB; [3]Institute of Medical Microbiology and Infection Control, University Hospital of Frankfurt, Frankfurt Am Main, Germany*

ThP 470 **Cancer Metabolome Dictates Susceptibility to Oncolytic Viral Therapy**; Barry Kennedy[1]; Patrick Murphy[1]; Michael Giacomantonio[1]; Prathyusha Konda[2]; Derek R Clements[1]; Namit Holay[1]; Shashi Gujar[1,2]; *[1]Department of Pathology, Dalhousie University, Halifax, NS, Canada, Halifax, NS; [2]Department of Microbiology and Immunology, Dalhousie University, Halifax, NS, Canada, Halifax, NS, Canada, Halifax, NS*

ThP 471 **HPLC-MS as a Detection Method for Pigments, Phenolics, and Co-Regulation in a Hybrid Wine Grape Family to Optimize Plant Breeding**; Abigail L Diering[1]; David Tork[1]; Dana Freund[1]; Matthew Clark[1]; Adrian Hegeman[1]; Anna Underhill[1]; *[1]University of Minnesota, St. Paul, MN*

ThP 472 **Cancer Cell Metabolism in KRAS Mice Revealed by Direct Sample Analysis with MALDI-TOF and High Resolution Mass Spectrometry**; Bo Wei[1]; Lin Tan[1]; Robyn Rhea[1]; Peiying Yang[1]; *[1]M D Anderson Cancer Center, Houston, TX*

ThP 473 **Characterization of Future Urine Reference Materials for the NIST Metabolomics Quality Assurance and Quality Control Program**; Abraham Kuri Cruz[1]; David A. Sheen[1]; Werickson F. C. Rocha[2]; Christina M. Jones[1]; *[1]National Institute of Standards and Technology, Gaitherburg, MD; [2]INMETRO, Duque De Caxias, Brazil*

ThP 474 **Database Assisted Globally Optimized Targeted Mass Spectrometry (dGOT-MS): Reliable Metabolomics Analysis with Broad Coverage**; Xiaojian Shi[1]; Haiwei Gu[1]; Paniz Jasbi[1]; *[1]Arizona State University, Scottsdale, AZ*

ThP 475 **How the Isotope Exchange Mass Spectrometry can Help Tandem Mass Spectrometry for Identification of Unknowns?**; Yury kostyukevich[1]; Alexander Zherebker[1]; Alexey orlov[1]; Eugene (evgeny) Nikolaev[2]; *[1]Skolkovo Institute of Science and Technology, Skolkovo, Russian Federation; [2]Skolkovo institute of science and technology, Moscow Region, Russian Federation*

ThP 476 **LC-HRMS Analysis of Small Molecules Formed in Cigarette Smoke-Exposed 3D Cellular Models Derived from Smokers and Non-Smokers**; Yuichiro Takanami[1]; Nobumasa Kitamura[1]; Shigeaki Ito[1]; *[1]Japan Tobacco Inc., Yokohama, Kanagawa, Japan*

ThP 477 **Rock Varnish as a Source of Biosignatures for Mars Extant Life**; Hiro Teshima[1]; Chris M Yeager[1]; Nina L Lanza[1]; Ricardo Marti-Arbona[1]; *[1]Los Alamos National Lab., Los Alamos, NM*

ThP 478 **An Integrated Ultra-High Resolution FTICR-MS based Platform for Metabolomics**; Yanlong Zhu[1]; Benjamin Wancewicz[1]; Kent Wenger[1]; Yutong Jin[1]; Heino M. Heyman[2]; Christopher J. Thompson[2]; Aiko Barsch[2]; Allan Brasier[1]; Ying Ge[1]; *[1]University of Wisconsin - Madison, madison; [2]Bruker Daltonics Inc., Billerica, MA*



METABOLOMICS: SAMPLE PREPARATION
479-482

ThP 479 **Metabolomics Links Doxycycline, Used Widely in Inducible Gene Silencing Experiments, with Metabolic Dysregulation in Breast Cancer Cells**; Ashish Vaswani; *Oregon State University, Corvallis, OR*

ThP 480 **Optimization of *C. elegans* Homogenization and Extraction Methods for LC-MS Untargeted Metabolomics**; Brianna M Garcia[1]; Bennett Fox[2,3]; Goncalo Gouveia[4]; Franklin E. Leach III[5]; Facundo M. Fernandez[6]; Frank Schroeder[2,3]; Arthur S. Edison[4]; I. Jonathan Amster[1]; *[1]Department of Chemistry, University of Georgia, Athens, GA; [2]Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY; [3]Boyce Thompson Institute, Ithaca, NY; [4]Department of Biochemistry, University of Georgia, Athens, Georgia; [5]Department of Environmental Health Science, University of Georgia, Athens, GA; [6]School of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA*

ThP 481 **On-Surface Derivatization Reactions for the High-Throughput Analysis of the Poultry Gut Microbiome using MALDI-MS**; Trevor T Forsman[1]; Torey Looft[2]; Young-Jin Lee[1]; *[1]Iowa State University, Ames, IA; [2]US Department of Agriculture, National Animal Disease Center, Ames, IA*

ThP 482 **Optimizing Methods to Extract Metabolites from Zebrafish Tissue**; Michaela Schwaiger-Haber[1]; Fuad J Naser[1]; Miriam Sindelar[1]; Jonathan L Spalding[1]; Gary J Patti[1]; *[1]Washington University, St. Louis, MO*

METABOLOMICS: UNTARGETED METABOLITE PROFILING III
483-512

ThP 483 **Interlaboratory Reproducibility of an Untargeted Metabolomics GC-MS Assay for Analysis of Human Plasma**; Yan-Ping Lin[1]; Ying Li[1]; Wen-sheng Lang[1]; John Masucci[1]; Gary W. Caldwell[1]; *[1]Janssen Research and Development, Spring House, PA*

ThP 484 **Establishing a Shareable Spectral MSMS Library and Accurate Mass Retention Time (AMRT) Database for Pediatric Metabolomics Analysis**; Chiara Lavarello[1]; Sebastiano Barco[1]; Anas Kamleh[2]; Igor Fochi[3]; Martina Bartolucci[1]; Gino Tripodi[1]; Giuliana Cangemi[1]; Andrea Petretto[1]; *[1]IRCCS Istituto Giannina Gaslini, Genova, Italy; [2]Thermo Fisher Scientific Europe, Hägersten, Sweden; [3]Thermo Fisher Scientific, Milano, Italy*

ThP 485 **Metabolic Characterization of Cell Clones in X. laevisEmbryos by HPLC-MS**; Jie Li[1]; Peter Nemes[1]; *[1]Department of Chemistry and Biochemistry, University of Maryland, College Park, MD*

ThP 486 **A Comprehensive N-Glycan Profiling Analysis of Bevacizumab Biosimilar by UHPLC with Fluorescence Detection and Q-TOF Mass Spectrometry**; Yonghai Lu[1]; Jie Xing[1]; Zhaoqi Zhan[1]; *[1]Shimadzu Asia Pacific, Singapore, Singapore*

ThP 487 **Discovery of Metabolite Biomarkers of Transition Period Diseases in Dairy Cows Using Chemical Isotope Labeling LC-MS**; Minglei Zhu[1]; Elda Dervishi[2]; Graham Plastow[2]; Marcos Colazo[3]; Liang Li[1]; *[1]University of Alberta, Edmonton, AB; [2]University of Alberta, Edmonton, Alberta; [3]Alberta and Agriculture Forestry, Edmonton, Alberta*

ThP 488 **Comprehensive Studies of Drug-induced Stemness of Cancer Cells at Single-cell Level**; Mei Sun[1]; Xingxiu Chen[1]; Zhibo Yang[1]; *[1]University of Oklahoma, Norman, OK*

ThP 489 **Comprehensive Untargeted Metabolite Identification with Kinetex F5 Microflow Liquid Chromatography and Variable Window Data Independent Acquisition**; Khatereh Motamedchaboki[1]; Remco van Soest[1]; Robert Proos[2]; Jason Anspach[3]; *[1]Sciex, Redwood City, CA; [2]Sciex, Framingham, MA; [3]Phenomenex, Torrance, CA*

ThP 490 **Multi-Feature Based Data Processing of Data Independent Acquisition (DIA) Metabolomics Data without Retention Time Information**; Pradeep Narayanaswamy[1]; Adam Iau[2]; Lyle Burton[2]; Stephen Tate[2]; *[1]Industry, Singapore, Singapore; [2]SCIEX, Concord, ON*

ThP 491 **Reacomics for LC-MS Based Untargeted Analysis**; Miao Yu[1,2]; Sofia Lendor[3]; Mariola Olkowicz[3]; Leslie Bragg[3]; Anna Roszkowska[3,4]; Mark Servos[3]; Janusz Pawliszyn[3]; *[1]University of Waterloo, Waterloo; [2]Icahn School of Medicine at Mount Sinai, New York, NY; [3]University of Waterloo, Waterloo, ON; [4]Medical University of Gdańsk, Gdańsk, Poland*

ThP 492 **Effect of a Mediterranean Based Diet on Plasma Metabolites**; Francis Briere[1]; Nancy Boucher[2]; Pier-Luc Plante[1]; Didier Brassard[1]; Simone Lemieux[1,3]; Benoit Lamarche[1,3]; Jacques Corbeil[1,2]; *[1]Universite Laval, Quebec, QC; [2]Infectiology Research Centre, CHU de Québec, Laval University, Québec, QC; [3]Institute of nutrition and functional foods, Université Laval, Québec, QC*

ThP 493 **Comprehensive Cell Culture Profiling of iPS Cell Using LC-QTOFMS: Simultaneous Analysis of SIM and Scan Mode in a Single Run**; Takanari Hattori[1]; Toshiya Matsubara[1]; Tsuyoshi Nakanishi[1]; Jun Watanabe[1]; *[1]Shimadzu Corporation, Kyoto, Japan*

ThP 494 **Multi-Omic Analysis of Macrophage and Macrophage Derived Exosomes with *Leishmania donovani* Infection**; Andrew P Kurland[1]; Vanessa Rubio[1]; Anna Gioseffi[1]; Peter Kima[1]; Timothy Garrett[1]; *[1]University of Florida, Gainesville, FL*

ThP 495 **Metabolomic Approach to Investigate Alteration in Metabolites Associated with 25-Hydroxyvitamin D in Healthy Korean Adults**; Mi-ri Gwon[1]; Bo Kyung Kim[1]; Seungil Cho[1]; Sook Jin Seong[1]; Young-ran Yoon[1]; *[1]Kyungpook National University, Daegu, South Korea*

ThP 496 **Investigation of Combined Tolcapone Metabolism and Brain Biochemistry Using an Integrated Human Multi-organ Microphysiological System**; Xin Wang[1]; Murat Cirit[1]; John Wishnok[1]; Linda Griffith[1]; Steven Tannenbaum[1]; *[1]Massachusetts Institute of Technology, Cambridge, MA*

ThP 497 **Beyond Aflatoxins: Untargeted Metabolic Profiling and Time Aligned Parallel fragmentation approach to Determine Gene Function in *A. flavus***; José Diana Di Mavungu[1]; Perng-Kuang Chang[2]; Leslie L. Scharfenstein[2]; Natalia Arroyo-Manzanares[3]; Valdet Uka[1]; Sarah De Saeger[1]; *[1]Ghent University, Ghent, Belgium; [2]US Department of Agriculture, Southern Regional Research Center, New Orleans, LA; [3]University of Murcia, Murcia, Spain*

ThP 498 **Application of Metabolite Derivatization for Simplication of Metabolomics Analysis by LC-MS**; Taylor F. Berryhill[1]; Landon S. Wilson[1]; Stephen Barnes[1]; *[1]University of Alabama at Birmingham, Birmingham, AL*

ThP 499 **Comparison and Evaluation of CCS Values Obtained via Direct Infusion IM-MS and LC-IM-MS for the Characterization of Rat Urine Metabolites**; Leanne Nye[1]; Jonathan P Williams[2]; Nyasha C Munjoma[2]; Marine PM Letertre[1]; Hernando J Olivos[3]; Muireann Coen[1]; Robbin Bouwmeester[4]; Lennart Martens[4]; Jeremy Nicholson[5]; Robert S Plumb[6]; Mike McCullagh[2]; Lee A Gethings[2]; Steven Lai[3]; James I Langridge[2]; Johannes PC Vissers[7]; Ian D Wilson[1]; *[1]Imperial College, London, United Kingdom; [2]Waters Corporation, Wilmslow, United Kingdom; [3]Waters Corporation, Beverly, MA; [4]Ghent University, Ghent, Belgium; [5]Murdoch University, Perth, Australia; [6]Waters Corporation, Milford, MA; [7]Waters Corporation, Wilmslow, United Kingdom*

ThP 500 **Intelligent Acquisition for Comprehensive Metabolome Coverage in Plants, Mammals, and Bacteria**; Tatjana D Talamantes[1]; Sven Hackbusch[2]; Ioanna Ntai[2]; Amanda

Souza[2]; [1]*Thermo Fisher Scientific, West Palm Beach, FL;* [2]*Thermo Fisher Scientific, San Jose, CA*

ThP 501 **Exploring Nematicidal Metabolites of Nematode-Trapping Fungi with LC-MS/MS-Based Untargeted Metabolomics;** Hsin-Yuan Chang[1]; Ting-Hao Kuo[1]; Ching-Ting Yang[2]; Yen-Ping Hsueh[2]; Cheng-Chih Hsu[1]; [1]*Department of Chemistry, National Taiwan University, Taipei, Taiwan;* [2]*Institute of Molecular Biology, Academia Sinica, Taipei, Taiwan*

ThP 502 **High-Throughput and Sensitive Data Independent Acquisition Workflow Differentiating Pre-Classified Healthy from Prediabetic and Diabetes Samples;** Khatereh Motamedchaboki[1]; Robert Proos[2]; Sara Ahadi[3]; Raghav Seghal[4]; Hemen Boro[4]; Abhishek Jha[4]; Latha Palaniappan[3]; [1]*Sciex, Redwood City, CA;* [2]*Sciex, Framingham, MA;* [3]*Stanford University, Palo Alto, CA;* [4]*Elucidata, Cambridge, MA*

ThP 503 **Using Quality Control Samples for Evaluating Quantification Reproducibility in Untargeted Metabolomics Based on Label-free and Chemical Isotope Labeling LC-MS;** Wei Han[1]; Shuang Zhao[1]; Liang Li[1]; [1]*University of Alberta, Edmonton, AB*

ThP 504 **Untargeted Metabolomic Analysis of Brain Sections Tissues from Mice with Low-Tryptophan Diet Using UHPLC-HRMS;** Frederico Garcia Pinto[1]; Vanessa Y. Rubio[2]; Gary P Wang[2]; Timothy J. Garrett[2]; [1]*Universidade Federal de Viçosa, Rio Paranaíba, Brazil;* [2]*University of Florida, Gainesville, FL*

ThP 505 **Rapid Detection of Drugs and Metabolites in Urine by Flow Injection Analysis Coupled to Magnetic Resonance Mass Spectrometry;** Matthias Witt[1]; Markus Godejohann[2]; Heino M. Heyman[3]; Alko Barsch[1]; [1]*Bruker Daltonik GmbH, Bremen, Germany;* [2]*Bruker Biospin GmbH, Rheinstetten, Germany;* [3]*Bruker Daltonics Inc., Billerica, MA*

ThP 506 **Metabolomics as a Discovery Tool for Bioprospecting and Detection of Defense Compounds During Fungal Infection of Spruce Wood;** Marit ALmvik[1]; Nina Elisabeth Nagy[1]; Hans Ragnar Norli[1]; Ari Hietala[1]; Sven-Roar Odenmarck[1]; Monica Fongen[1]; Anas M Kamleh[2]; [1]*Norwegian Institute of Bioeconomy Research (NIBIO), Oslo, Norway;* [2]*Thermo Fisher Scientific Europe, Hagersten, Sweden*

ThP 507 **Biological Signal Averaging and PLSDA Variable Statistics in a High-Yield Drought-Tolerant Maize Transgene vs. Wildtype High-Throughput GC-MS Plant Metabolomics Experiment;** Brian M. Ruddy[1]; Teresa K. Harp[1]; Layton A. Peddicord[1]; Shai J. Lawit[1]; Jingrui Wu[1]; Jeffrey E. Habben[1]; Jan P. Hazebroek[1]; [1]*Corteva Agriscience, Johnston, IA*

ThP 508 **Assessing the Bioactivity of Environmental Surface Waters by Metabolomics Using Multiple Cell Lines;** Yang Yue[1]; Jonathan Mosley[1]; Paul Bradley[2]; Jenna Cavallin[3]; Daniel Villeneuve[3]; Gerald Ankley[3]; Drew Ekman[1]; Timothy Collette[1]; Quincy Teng[1]; [1]*U.S. Environmental Protection Agency, Athens, GA;* [2]*U.S. Geological Survey, Columbia, SC;* [3]*U.S. Environmental Protection Agency, Duluth, MN*

ThP 509 **Challenges of Data Acquisition for Large Set of Untargeted Metabolomics Studies;** Linxing Yao[1]; Tove Fall[2]; Erik Ingelsson[3]; Lars Lind[4]; Jessica E. Prenni[5]; Amy M Sheflin[5]; Corey D. Broeckling[1]; [1]*Proteomics & Metabolomics Facility, Colorado State University, Fort Collins, CO;* [2]*Department of Medical Sciences, Molecular Epidemiology and Science for Life Laboratory, Uppsala University, Uppsala, Sweden;* [3]*School of Medicine, Stanford University, Stanford, CA;* [4]*Department of Medical Sciences, Cardiovascular Epidemiology, Uppsala University,, Uppsala, Sweden;* [5]*Department of Horticulture and Landscape Architecture, Colorado State University, Fort Collins, CO*

ThP 510 **Using Metabolomics to Assess Physiological Changes Accompanying Cyanide Metabolism in *Pseudomonas fluorescens* NCIMB 11764;** Prajita Pandey[1]; Lauren Jones[1]; Daniel A. Kunz[1]; Vladimir Shulaev[1]; [1]*University of North Texas, Denton, TX*

ThP 511 **GC-MS Profiling of Soy-Induced Correlated Changes in the Fecal Metabolome and Gut Microbiome of Ovariectomized Female Rats;** Saurav J Sarma[1, 2]; Victoria J Vieira-Potter[3]; Tzu-Wen L Cross[4]; Kelly S Swanson[5, 6]; Zhentian Lei[1, 2, 7]; Lloyd W Sumner[1, 2, 7]; Cheryl S Rosenfeld[2, 8, 9, 10]; [1]*Metabolomics Center, University of Missouri, Columbia, MO;* [2]*Bond Life Sciences Center, University of Missouri, Columbia, MO;* [3]*Department of Nutrition and Exercise Physiology, University of Missouri, Columbia, MO;* [4]*Department of Bacteriology, University of Wisconsin-Madison, WI, Madison, WI;* [5]*Division of Nutritional Sciences, University of Illinois at Urbana-Champaign, Urbana, IL;* [6]*Department of Animal Sciences, University of Illinois at Urbana-Champaign, Urbana, IL;* [7]*Department of Biochemistry, University of Missouri, Columbia, MO;* [8]*Biomedical Sciences, University of Missouri, Columbia, MO;* [9]*Thompson Center for Autism and Neurobehavioral Disorders, University of Missouri, Columbia, MO;* [10]*Genetics Area Program, University of Missouri, Columbia, Columbia, MO*

ThP 512 **Quantitative Evaluation of Untargeted Metabolomic Methods for Zebrafish Blood;** Fuad J Naser[1]; Ronald Fowle-Grider[1]; Kevin Cho[1]; Jonathan L Spalding[1]; Gary J Patti[1]; [1]*Washington University in St. Louis, St. Louis, MO*

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ThP 513 **Typing of emm1 Group A Hemolytic Streptococci Using MALDI-TOF MS;** Megumi Sakuma[1]; Keisuke Shima[2]; Shinji Funatsu[2]; Koretsugu Ogata[2]; Miyuki Morozumi[1]; Satoshi Iwata[1]; [1]*Keio University School of Medicine, Shinjuku-ku, Japan;* [2]*SHIMADZU, Kyoto, Japan*

ThP 514 **MALDI-MS Proteotyping of Cutibacterium acnes;** Kanae Teramoto[1]; Tatsuki Okubo[1]; Yoshihiro Yamada[1]; Sadanori Sekiya[1]; Shinichi Iwamoto[1]; Koichi Tanaka[1]; [1]*Shimadzu Corporation, Kyoto, Japan*

ThP 515 **Epigenetic "Memory" During Bacterial Adaptation to Environmental Changes;** Alena Calm[1]; Gabrielle Rizzo[2]; Trevor Glaros[1]; Henry S Gibbons[1]; [1]*ECBC, Aberdeen Proving Ground, Maryland;* [2]*ECBC, Excet Contractor, Aberdeen Proving Ground, Maryland*

ThP 516 **Improved MALDI-MS method in stability and reproducibility of peak detection of the biomarkers for proteotyping of Salmonella serotypes;** Yuko Fukuyama[1]; Teruyo Ojima-Kato[2]; Satomi Nagai[2]; Keisuke Shima[1]; Shinji Funatsu[1]; Yoshihiro Yamada[1]; Hiroto Tamura[2]; Shizuo Nomura[1]; Koretsugu Ogata[1]; Sadanori Sekiya[1]; Shinichi Iwamoto[1]; Koichi Tanaka[1]; [1]*Shimadzu Corporation, Kyoto, Japan;* [2]*Meijyo University, Nagoya, Japan*

ThP 517 **Chemical Changes On, and through, the Bacterial Envelope in *E. coli* Mutants Exhibiting Impaired Plasmid Transfer Identified Using ToF-SIMS;** kelly Dimovska Nilsson[1]; John Fletcher[1]; [1]*University of Gothenburg, Gothenburg, Sweden*

ThP 518 **Electroporation and LESA-MS: A New Paradigm for Top-Down Analysis of Proteins Direct from Living Yeast Colonies;** Klaudia I Kocurek[1, 2]; Robin C May[1]; Helen J Cooper[1]; [1]*University of Birmingham, Birmingham, United Kingdom;* [2]*Texas A&M University, College Station, TX*

ThP 519 **Keeping it Clean: Metaproteomic Characterization of a Microbiome Capable of Degrading Personal Care Product and Pharmaceutical Contaminants found in Water;** Kitty J. Brown[1]; Karen E. Rossmassler[2]; Lisa M Wolfe[1]; Parker J. Muck[1]; Jean F. Challacombe[3]; Jessica E. Prenni[4]; Susan K. De Long[5]; Corey D. Broeckling[1]; [1]*Proteomics & Metabolomics Facility, Colorado State*



University, Fort Collins, CO; [2]Pulmonary Section, Denver Veterans Affairs Medical Center; Division of Pulmonary Sciences & Critical Care Medicine, University of Colorado Denver, Denver, CO; [3]College of Agricultural Sciences, Colorado State University, Fort Collins, CO; [4]Department of Horticulture & Landscape Architecture, Colorado State University, Fort Collins, CO; [5]Department of Civil & Environmental Engineering, Colorado State University, Fort Collins, CO

ThP 520 **Model Based Spectral Library for Bacterial Identification *via* Membrane Glycolipids**; So Young Ryu[1]; George A. Wendt[1,2]; Robert K. Ernst[3]; David R. Goodlett[3]; *[1]University of Nevada, Reno, NV; [2]University of California, Berkeley, CA; [3]University of Maryland, Baltimore, MD*

ThP 521 **The *Trichomonas vaginalis* Cytoskeletal Proteome**; Katherine Muratore[1]; Patricia Johnson[1]; *[1]University of California Los Angeles, Los Angeles, CA*

ThP 522 **HAMA: High-Throughput Automated Muropeptide Analysis Framework for Revealing Composition of Bacterial Peptidoglycan**; Pin-Rui Su[1,2]; Ya-Chen Hsu[1]; Hsin-Hsiang Chung[1]; Yun Lin[1]; Tsuey-Ching Yang[3]; Cheng-Chih Hsu[1]; *[1]National Taiwan University, Taipei, Taiwan; [2]Erasmus MC, Rotterdam, Netherlands; [3]National Yang-Ming University, Taipei, Taiwan*

ThP 523 **Typing Environmental Microorganisms To Genomic Databases Using MALDI Mass Spectrometry**; Kenneth C. Parker; *SimulTOF/ VIC Instruments, Marlborough, MA*

ThP 524 **Characterization of Lysine Acetylation in Human Gut Microbiome**; Xu Zhang[1]; Zhibin Ning[1]; Janice Mayne[1]; Shelley Deeke[1]; Krystal Walker[1]; David Mack[2]; Alain Stintzi[1]; Daniel Figeys[1]; *[1]University of Ottawa, Ottawa, ON; [2]Children's Hospital of Eastern Ontario, Ottawa, ON*

ThP 525 **Top Down Protein Identification of ESKAPE Pathogens from *in vitro* Skin Models and *ex vivo* Human Skin by LESA MS**; Jana Havlikova[1,2]; Robin C. May[2,3]; Iain B. Styles[4]; Helen J. Cooper[2]; *[1]EPSRC Centre for Doctoral Training in Physical Sciences for Health, University of Birmingham, Birmingham, United Kingdom; [2]School of Biosciences, University of Birmingham, Birmingham, United Kingdom; [3]Institute of Microbiology and Infection, University of Birmingham, Birmingham, United Kingdom; [4]School of Computer Science, University of Birmingham, Birmingham, United Kingdom*

ThP 526 **Cell-Free Identification of *S. cerevisiae* Strains Used in Beer Production using LC-MS**; Cathy Muste[1]; Kevin Owens[1]; *[1]Drexel University, Philadelphia, PA*

ThP 527 **Integrated, Multi-Omics Strategy to Study the Gut Microbiota Response to Salmonella enterica Typhimurium Infection In Humanized Mice**; Pingli Wei[1]; Caitlin Keller[1]; Jennifer R. Bratburd[2]; Rui Liu[3]; Eugenio Vivas[2]; Erin Gemperline[1]; Federico E. Rey[2]; Cameron R. Currie[2]; Lingjun Li[1,4]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]Department of Bacteriology, University of Wisconsin-Madison, WI, Madison, WI; [3]School of Pharmacy, Nanjing University of Chinese Medicine, Nanjing, China; [4]School of Pharmacy, University of Wisconsin-Madison, Madison, WI*

ThP 528 **Characterization of Novel Assembly Mechanisms of a Large Viral Icosahedral Capsid**; Erin Reilly[1]; Zein Haidar[1]; Ru-ching Hsia[2]; Sammy Pardo[3]; Dana Molleur[3]; Susan T. Weintraub[3]; Julie A. Thomas[1]; *[1]Rochester Institute of Technology, Rochester, NY; [2]University of Maryland School of Dentistry, Baltimore, MD; [3]University of Texas Health Science Center at San Antonio, San Antonio, TX*

ThP 529 **Molecular Networking Guided Profiling of Metabolic Pathways in Engineered Microorganisms for Industrial Production of Chemical Intermediates**; Alexey V. Melnik[1]; Bryan Fonslow[1]; Ali Khodayari[1]; Julia Khandurina[1]; Pieter C. Dorrestein[2]; *[1]Genomatica Inc., San Diego, CA; [2]UCSD, La Jolla, CA*

ThP 530 **Examining the Discrimination Power of MAI, vMAI, and SAI for Identification of Microorganisms**; Darrell D. Marshall[1,2]; Santosh Karki[1,2]; Khoa Hoang[1,3]; Milan Pophristic[1,3]; Chuping Lee[2]; Ellen Inutan[1,4]; Samantha Leach[5]; Charles N McEwen[1,3]; Sarah Trimpin[1,2]; *[1]MSTM, LLC, Newark, DE; [2]Wayne State University, Detroit, MI; [3]University of the Sciences, Philadelphia, PA; [4]MSU-Iligan Institute of Technology, Illigan City, Philippines; [5]Department of Forensic Sciences, Washington, DC*

ThP 531 **Time-Dependent Analysis of *Paenarthrobacter nicotinovorans* pAO1 Nicotine-Related Proteome**; Marius Mihasan[1]; Cornelia Babii[1]; Devika Channaveerappa[2]; Roshanak Aslebagh[2]; Emmalyn Dupree[2]; Costel C Darie[2]; *[1]Alexandru Ioan Cuza University of Iasi, Iasi, Romania; [2]Clarkson University, Potsdam*

ThP 532 **Real-time, Automated Characterization of Algal Lipidome and Metabolome Using Laser-Assisted Rapid Evaporative Ionization Mass Spectrometry**; Julia Balog[1,2]; Richard Schäffer[1]; Milan Szabo[3,4]; Unnikrishnan Kuzhiumparambil[3]; Steven D Pringle[5]; Peter Ralph[3]; Zoltan Takats[2]; *[1]Waters Research Center, Budapest, Hungary; [2]Imperial College, London, United Kingdom; [3]University of Technology Sydney, Sydney, Australia; [4]Biological Research Centre of the Hungarian Academy of Sciences, Szeged, Hungary; [5]Waters Corporation, Wilmslow, United Kingdom*

ThP 533 **MS-Based Metaproteomics Can Be Integrated with Metagenome Assembled Genomes to Provide Genome Specific Protein Identification in Gut Microbiomes**; Jose Alfredo Blakeley-Ruiz[1]; Carlee S McClintock[2]; Richard J. Giannone[3]; Helen A Baghdoyan[1]; Ralph Lydic[1]; Mircea Podar[3]; Robert L. Hettich[3]; *[1]University of Tennessee, Knoxville, TN; [2]Pain Consultants of East Tennessee, Knoxville, Tennessee; [3]Oak Ridge National Laboratory, Oak Ridge, TN*

ThP 534 **Characterization of Microorganisms by Proteins and Lipids MALDI-TOF Fingerprints: Case Studies**; Vincent Guérineau[1]; Morgane Barthélemy[1]; Marceau Levasseur[1]; Téo Hébra[1]; Véronique Eparvier[1]; David Touboul[1]; *[1]CNRS-ICSN, Gif Sur Yvette, France*

ThP 535 **Distinguishing Bacteria from Near Neighbors by Paper Spray Mass Spectrometry**; Daniel Carmany[1]; Ethan M McBride[2]; Phillip Mach[2]; Elizabeth S Dhummakupt[2]; Paul S Demond[1]; Gabrielle Rizzo[1]; Nicholas E Manicke[3]; Trevor Glaros[2]; *[1]Excet, Inc., Springfield, VA; [2]ECBC, Aberdeen Proving Ground, Maryland; [3]IUPUI Department of Chemistry & Chemical Biology, Indianapolis, IN*

ThP 536 **Typing/Subtyping Shiga Toxin from Pathogenic *Escherichia coli* Using MALDI-TOF-TOF Tandem Mass Spectrometry and Top-Down Proteomic Analysis**; Clifton K. Fagerquist[1]; William J. Zaragoza[1]; Michelle Q. Carter[1]; *[1]USDA/ ARS, Albany, CA*

ThP 537 **Developing Sample Preparation Conditions to Analyze a Remarkably Resilient Protein Assembly, the Methanosaeta concilii Sheath**; John Muroski[1]; Farzaneh Sedighian[1]; Robert P. Gunsalus[1]; Joe A Loo[1]; Rachel R Orgazalek Loo[1]; *[1]UCLA, Los Angeles, CA*

ThP 538 **Influence of Phage SPN3US Infection on the Salmonella Host Proteome**; Caleb Emmons[1]; Julie A. Thomas[2]; Susan Ludwigsen[1]; Jimar Miller[1]; Sammy Pardo[3]; Dana Molleur[3]; Susan T. Weintraub[3]; *[1]Proteome Software, Portland, OR; [2]Rochester Institute of Technology, Rochester, NY; [3]University of Texas Health Science Center at San Antonio, San Antonio, TX*

ThP 539 **Microbial Synthesis of a Novel Vitamin B9 Derivative and its Immunomodulatory Impact**; Abby J. Chiang[1]; Daniel Röth[1]; Anne E. Hall[2]; Gabriel B Gugiu[1]; James Versalovic[2,3]; Markus Kalkum[1]; *[1]City of Hope, Duarte, CA; [2]Baylor College of Medicine, Houston, Texas; [3]Texas Children's Hospital, Houston, Texas*

ThP 540 **Evidence of Sodium Substitution for Hydrogen in Negative Ion Lipid A Tandem Mass Spectra of *Burkholderia thailandensis***; Sung Hwan Yoon[1,2]; Courtney E. Chandler[1]; Inga V. Leus[3]; Aleksandra Nita-lazar[2]; Helen I. Zgurskaya[3]; David R. Goodlett[1]; Robert K. Ernst[1]; *[1]University of Maryland, Baltimore, MD; [2]NIH/NIAID, Bethesda, Maryland; [3]University of Oklahoma, Norman, OK*

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ThP 541 **9.4 T FT-ICR Mass Spectrometer with Cluster Ion Source for Analysis of Molecular Nanocarbons**; Paul Dunk[1]; Yuri E. Corilo[1]; Christopher L. Hendrickson[1]; *[1]National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL*

ThP 542 **Rapid Determination of Progestogens by Solid-Phase Extraction with Functionalized Metal-Organic Frameworks Coupled to Direct Analysis in Real Time Mass Spectrometry**; Linnan Li[1]; Yuangui Yang[1]; Mei Tian[1]; Ruirong Zheng[1]; Li Yang[1,2]; Zhengtao Wang[1,2]; *[1]Shanghai University of Traditional Chinese Medicine, Shanghai, China; [2]Shanghai R&D Center for Standardization of Chinese Medicines, Shanghai, China*

ThP 543 **Preparation of Gas Phase Naked Silver Cluster Cations Outside a Mass Spectrometer from Ligand Protected Clusters in Solution**; Madhuri Jash[1]; Arthur C. Reber[2]; Atanu Ghosh[1]; Depanjan Sarkar[1]; Mohammad Bodiuzzaman[1]; Pallab Basuri[1]; Ananya Baksi[1]; Shiv N. Khanna[2]; Thalappil Pradeep[1]; *[1]Indian Institute of Technology, Madras, Chennai, India; [2]Virginia Commonwealth University, Richmond, VA*

ThP 544 **Top-Down Phosphoproteomics Enabled by Novel Nanoproteomics Platform**; David S Roberts[1]; Bifan Chen[1]; Timothy N. Tiambeng[1]; Zhijie Wu[1]; Ying Ge[1,2,3]; Song Jin[1]; *[1]Department of Chemistry, University of Wisconsin-Madison, Madison, WI; [2]Department of Cell and Regenerative Biology, University of Wisconsin-Madison, Madison, WI; [3]Human Proteomics Program, School of Medicine and Public Health, University of Wisconsin-Madison, Madison, WI*

ThP 545 **Determination of Molecular and Topographical Organization on Cicada Wings: Mass Spectrometry's Impact on Material Characterization and Design**; Jessica K Román[1,2]; Jacob B Hoffman[2]; Julian H Reed[2]; Nenad Miljkovic[3]; Donald M Cropek[2]; Marianne Alleyne[3]; *[1]Sandia National Laboratories, Albuquerque, NM; [2]US Army Corps of Engineers, Champaign, IL; [3]University of Illinois at Urbana Champaign, Urbana, IL*

ThP 546 **Neutrophil Extracellular Trap Formation in the Lung as Response to Magnetic Cobalt Ferrite Nanoparticles**; Anja M Billing[1]; Kristina B Knudsen[2]; Håkan Wallin[3]; Selina VY Tang[4]; Iseult Lynch[5]; Ulla Vogel[3,6]; Frank Kjeldsen[1]; *[1]Department of Biochemistry and Molecular Biology, University of Southern Denmark, Odense, Denmark; [2]National Research Centre for the Working Environment, Copenhagen, Denmark; [3]National Research Centre for the Working Environment, Copenhagen, Denmark; [4]Promethean Particles, Nottingham, United Kingdom; [5]School of Chemistry and Chemical Biology, University College Dublin, Dublin, Ireland; [6]Department of Micro- and Nanotechnology, Technical University of Denmark, Lyngby, Denmark*

ThP 547 **Pre-Adsorption of Antibodies on Nanocarriers: Retaining Targeting Properties in a Complex Protein Environment**; Johanna Simon[1]; Manuel Tonigold[2]; Katharina Landfester[1]; Volker Mailänder[1,2]; *[1]Max Planck Institute for Polymer Research, Mainz, Germany; [2]University of Mainz, Mainz, Germany*

ThP 548 **Complementary Molecular Profiling of Neuropeptides and Lipids from Lymnaea stagnalisby LDI-Mass Spectrometry on Matrix-Assisted and Silicon Nanopost Array Platforms**; Ellen A Wood[1]; Sylwia A Stopka[1]; Akos Vertes[1]; *[1]The George Washington University, Washington, DC*

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ThP 549 **Method for Detecting of the Ratio of Tannic Acid-Metal Complex by Nano-Electrospray Ionization Mass Spectrometry**; Rui Chen; *Yunnan Normal University, Kunming, China*

ThP 550 **The Dynamic Sampling Platform (DSP) for ESI-MS Monitoring of Bioreactors for Therapeutic Cell Manufacturing**; Mason A Chilmonczyk[1]; Gian C Rivera[2]; Peter A Kottke[1]; Robert E Guldberg[3]; Andrei G Fedorov[1]; *[1]Georgia Institute of Technology, Atlanta, GA; [2]University of Puerto Rico - Mayagüez, Mayagüez, PR; [3]University of Oregon, Eugene, OR*

ThP 551 **Deep and Sensitive Proteomics Using Capillary Electrophoresis-Mass Spectrometry with the Identification of 7000 Proteins from nanograms of MCF7 Proteome Digests**; Zhichang Yang[1]; Xiaojing Shen[1]; Daoyang Yang[1]; Liangliang Sun[1]; *[1]Michigan State University, East Lansing*

ThP 552 **Extending the Lower Limits of Quantification of a Therapeutic Oligonucleotide through Microflow LC-MS/MS**; Daniel Warren[1]; Sean McCarthy[2]; Lei Xiong[3]; Anthony Romanelli[2]; *[1]AB SCIEX, Framingham; [2]Sciex, Framingham, MA; [3]Sciex, Redwood City, CA*

ThP 553 **Water and Temperature-Assisted Trap Focusing for Ultra-Large Volume Injection in Reversed-Phase Nano-Liquid Chromatography Mass-Spectrometry**; Veronica Termopoli[1]; Pierangela Palma[1]; Giorgio Famiglini[1]; Gian Luca Morini[2]; Pamela Vocale[3]; Mansoor Saeed[4]; Simon Perry[4]; Achille Cappiello[1]; *[1]University of Urbino, Urbino, Italy; [2]University of Bologna, Bologna, Italy; [3]University of Parma, Parma, Italy; [4]Syngenta Jealott's Hill International Research Centre, Bracknell, United Kingdom*

ThP 554 **ESI-MS Intracellular Metabolite Profiling for Therapeutic Cell Manufacturingvia Microfabricated Mass Exchanger**; Austin L Culberson[1]; Mason A Chilmonczyk[1]; Peter A Kottke[1]; Andrei G Fedorov[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

ThP 555 **Rapid Characterization of Recombinant Protein Processing Using Microchip-Based Capillary Electrophoresis-ESI-MS**; David McCaskill[1]; Vimbai Chikwana[1]; Jeffrey Gilbert[1]; *[1]Corteva Agriscience, Indianapolis, IN*

ThP 556 **High-Sensitivity Glycomic and Proteomic Profiling of Limited Biological Samples Using Capillary Zone Electrophoresis-Mass Spectrometry**; Anne-Lise Marie[1]; Kendall Johnson[1]; Marcia Santos[2]; Somak Ray[1]; Antonius Koller[1]; David Frank[3]; Helen Gandler[3]; Shulin Lu[3]; John Tigges[3]; Ionita Ghiran[3]; Alexander R Ivanov[1]; *[1]Northeastern University, Boston, MA; [2]Sciex, Brea, CA; [3]Harvard Medical School, boston, MA*

ThP 557 **Microchip Capillary Electrophoresis-Negative Electrospray Ionization-Mass Spectrometry for High Sensitivity Anion Detection**; Yury Desyaterik[1]; Jean Pierre Alarie[1]; J. Michael Ramsey[1]; *[1]UNC, Chapel Hill, NC*

ThP 558 **Monitoring Amino Acid Composition of Cell Culture Media using Microfluidic CE-MS**; Erin Redman[1]; Kathryn Elliot[2]; Cameron Schnabel[2]; Sarah Harcum[2]; J. Scott Mellors[1]; Glenn Harris[3]; *[1]908 Devices, Inc., Carrboro, NC; [2]Department of Bioengineering, Clemson University, Clemson, SC; [3]908 Devices, Boston, MA*

ThP 559 **Multilevel Characterization and Identification of Trastuzumab Posttranslational Modifications by Imaged cIEF-MS**; Erik Gentalen[1]; Steve Lacy[1]; Jennifer Ji[1]; Lena Wu[1]; Scott Mack[1]; *[1]Intabio, Inc., Newark, CA*

ThP 560 **High-Sensitivity Analysis of Durgs in Ultra-Small Volumes Plasma Samples using Micro-Flow LC-MS/MS**; Davide Vecchietti[1]; Mikaël Levi[1]; Hidetoshi Terada[1]; Jonathan Edwardsen[2]; Keiko Matsumoto[1]; Kyoko Watanabe[1]; Masami Tomita[1]; *[1]Shimadzu Corporation, Kyoto, Japan; [2]Shimadzu Scientific Instruments, Inc., Columbia, Maryland*

ThP 561 **Integrating Nanofluidic/Microfluidic Interface Concentrators/Microreactor with ESI-MS for Proteome Analysis**; Dayi Chen[1]; Kantaphon Suddhapas[1]; Timothy J Fogliatti[1]; Aaron T Timperman[1]; *[1]University of Illinois Urbana-Champaign, Urbana, IL*

ThP 562 **In-syringe ElectrokineticClean-up of Weakly Acidic Drugs in Biological Samples for Direct Injection Electrospray Ionization Mass Spectrometry**; Ibraam E Mikhail[1, 2, 3]; Masoomeh Tehranirokh[1, 4]; Andrew A Gooley[1, 4]; Rosanne M Guijt[1, 5]; Michael C Breadmore[1, 2]; *[1]ARC Training Centre for Portable Analytical Separation Technologies (ASTech), Hobart, Australia; [2]Australian Centre for Research on Separation Science (ACROSS), School of Physical Sciences (Chemistry), University of Tasmania, Hobart, Australia; [3]Department of Analytical Chemistry, Faculty of Pharmacy, Mansoura University, Mansoura, Egypt; [4]Trajan Scientific and Medical, Ringwood, Australia; [5]Centre for Regional and Rural Futures, Deakin University, Geelong, Australia*

ThP 563 **High-Throughput Proteome Analysis Using 50 cm Long Micro Pillar Array Columns (µPACTM)**; Jeff Op De Beeck[1]; Geert Van Raemdonck[1]; Paul Jacobs[1]; Gert Desmet[2]; Wim De Malsche[2]; Francis Impens[3]; Kris Gevaert[3]; *[1]PharmaFluidics, Ghent, Belgium; [2]Vrije Universiteit Brussel, Brussels, Belgium; [3]VIB-UGent Center for Medical Biotechnology, Ghent, Belgium*

ThP 564 **Microchip Integration of Imaged cIEF with Mass Spectrometry Accelerates the Identification of Charge Variants in Intact Monoclonal Antibodies**; Scott Mack[1]; Steve Lacy[1]; Jennifer Ji[1]; Guillaume Tremintin[2]; Lena Wu[1]; Erik Gentalen[1]; *[1]Intabio, Inc., Newark, CA; [2]Bruker Daltonics Inc., Billerica, MA*

ThP 565 **Analysis of Peptides Using Nano LC with Micro Pillar Array Columns (µPAC™) and Microsaic Real-Time 4500 MiD® Mass Spectrometer**; Victoria Ordsmith[1]; Bin Chen[1]; Chris Harris[1]; *[1]Microsaic Systems, Woking, United Kingdom*

ThP 566 **Ultra-Sensitive Deep LC-MS Proteomic Profiling Using Ultra-Low Flow Monolithic and Porous-Layer Open Tubular Capillary Columns**; Michal Gregus[1]; Antonius Koller[1]; Alexander R Ivanov[1]; *[1]Northeastern University, Boston, MA*

NATURAL PRODUCTS
567-589

ThP 567 **Cytochrome P450 Inhibition by Licorice *Glycyrrhiza uralensis* Fisch. ex DC.**; Luying Chen[1, 2]; Laura Tyler[2]; Dejan Nikolic[2]; Guido F. Pauli[2]; Richard B. van Breemen[1, 2]; *[1]Linus Pauling Institute, College of Pharmacy, Oregon State University, Corvallis, OR; [2]UIC/NIH Center for Botanical Dietary Supplements Research, Chicago, IL*

ThP 568 **Unequivocal identification of alkylpyrazines by Gas Chromatography-Mass Spectrometry (GC-MS)**; Sihang Xu[1]; Athula Attygalle[1]; Ramu Errabelli[2]; *[1]Stevens Institute of Technology, Hoboken, NJ; [2]SGS New Jersey laboratory, Fairfield, NJ*

ThP 569 **Automation and Application of Magnetic Based Affinity Selection Screening for Targets of Retinoid X Receptor alpha (RXRα)**; Ruth N Muchiri[1]; Jaewoo Choi[1]; Katherine A Carter[1]; Brett M Tyler[1]; Richard B. van Breemen[1]; *[1]Oregon State University, Corvallis, OR*

ThP 570 **PepSAVI-MS Reveals a Novel Antimicrobial Peptide from Amaranth**; Lilian R. Heil[1]; Tessa E. Bartges[1]; Christine L. Kirkpatrick[1]; Nicole C. Parsley[1]; Dennis Goldfarb[2]; Leslie M Hicks[1]; *[1]Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]Department of Cell Biology and Physiology, Lineberger Comprehensive Cancer Center, University of North Carolina at Chapel Hill, Chapel Hill, NC*

ThP 571 **Finding Alkaloids in Plant Extracts by LC-QToF Mass Spectrometry in Combination with Mass Defect Analysis**; Armando Alcazar Magana[1, 2]; Bayissi Bading-Taika[3]; Jaewoo Choi[1]; Cristobal L. Miranda[1]; Claudia S. Maier[2]; Jan F. Stevens[1]; *[1]Linus Pauling Institute, College of Pharmacy, Oregon State University, Corvallis, OR; [2]Department of Chemistry, Oregon State University, Corvallis, Oregon; [3]Department of Clinical and Pharmaceutical Sciences, School of Life and Medical Sciences, University of Hertfordshire, Hertfordshire, United Kingdom*

ThP 572 **LC-MS-Based Analysis of Antimicrobial Compounds Produced by *Streptomyces coelicolor* Harboring Metagenome-Derived Biosynthetic Gene Clusters** ; Angela I Calderon[1]; Megan Sandoval-Powers[1]; Yilue Zhang[1]; Hannah Kim[1]; Alinne Santana-Pereira[1]; Mark Liles[1]; David Mead[2]; *[1]Auburn University, Auburn, Alabama; [2]Varigen Biosciences Corporation, Madison, WI*

ThP 573 **Ozone-Induced Dissociation Mass Spectrometry as a New Tool to Determine the C=C Double Bond Locations in Natural Products**; Ngoc Vu[1]; Sonja Knowles[1]; Nicholas Oberlies[1]; Qibin Zhang[1, 2]; *[1]UNC Greensboro, Greensboro, NC; [2]Center for Translational Biomedical Research, Kannapolis, NC*

ThP 574 **LC-MS-Based Chemical Characterization of Constituents of Açaí Methanol Extract and Metabolites Obtained from an *in vitro* Intestinal First-Pass Metabolism Study**; Yilue Zhang[1]; Turner Shirley[1]; Tyler Wietlake[1]; Richard A. Hansen[2]; Jingjing Qian[2]; Angela I. Calderon[1]; *[1]Department of Drug Discovery and Development, Auburn University, Auburn, AL; [2]Department of Health Outcomes Research and Policy, Auburn University, Auburn, AL*

ThP 575 **LC-HRMS followed by Enhanced Product Ion Scanning for Flavonoids Profiling of Primula boveana**; Ehab Mahran[1, 2]; Michael Keusgen[1]; *[1]Institute of Pharmacy, Philipps-Universität Marburg, Marburg, Germany; [2]Faculty of Pharmacy, Al-Azhar University, Nasr city, Egypt*

ThP 576 **Identification of Biofilm-Stimulating Peptides from *Bacillus cereus* with PepSAVI-MS**; Tessa E. Bartges[1]; Steven R. Fleming[1]; Sarah A. Barr[1]; Elizabeth A. Shank[1]; Albert A. Bowers[1]; Leslie M. Hicks[1]; *[1]University of North Carolina, Chapel Hill, NC*

ThP 577 **Determination and Visualization of Components from a Medical Fungus Using High-Performance Liquid Chromatography Mass Spectrometry and Imaging Mass Spectrometry**; Jing Dong[1]; Satoshi Yamaki[1]; Xiaodong Li[1]; Naoki Hamada[1]; *[1]SHIMADZU CHINA MS CENTER, Beijing, China*

ThP 578 **Using Ozone Induced Dissociation Mass Spectrometry (OzID-MS) for Natural Product Analysis: Pure Compound, Complex Extract, and *in situ***; Sonja L. Knowles[1]; Ngoc Vu[1]; Daniel A. Todd[1]; Huzefa A. Raja[1]; Antonis Rokas[2]; Qibin Zhang[1, 3]; Nicholas H. Oberlies[1]; *[1]University of North Carolina at Greensboro, Greensboro, NC; [2]Vanderbilt University, Nashville, TN; [3]Center for Translational Biomedical Research, Kannapolis, NC*

ThP 579 **Isolation and Identification of Naphthomycins Production by Actinomycetes as Antifungal Compounds against *Colletotrichum acutatum***; Fernando L.S. Fugita[1]; Nicolas L. M. Freiria[1]; Luiz A.B. Moraes[1]; *[1]Faculty of Philosophy, Sciences and Letters at Ribeirao Preto (USP), Ribeirão Preto, Brazil*

ThP 580 **Bacteria Fight Club: Mapping Microbial Interactions for Drug Discovery**; Berkley Ellis[1]; Caleb N Fischer[1]; Brian

O Bachmann[1]; John A. McLean[1]; [1]*Vanderbilt University, Nashville, TN*

ThP 581 **Analysis of Diterpenoids in *Tripterygium wilfordii* by Supercritical Fluid Chromatography Coupling Tandem Mass Spectrometry**; Lingna Ke[1]; Ming Yuan[2]; Qing Fu[1]; Zhengwei Jia[2]; Yu Jin[1]; [1]*East China University of Science and Technology, Shanghai, China;* [2]*Waters Technologies (Shanghai) Co., Ltd, Shanghai, China*

ThP 582 **Modulation of the Secondary Metabolites Production in Streptomyces Caat 8-25 under Metal Stress by LC-MS/MS**; Talita C. T. Medeiros[1]; Bruna B. Loiola[1]; Luiz A.B. Moraes[1]; [1]*Faculty of Philosophy, Sciences and Letters at Ribeirao Preto (USP), Ribeirão Preto, Brazil*

ThP 583 **Determination of Artemisinin and Its Precursors in *Artemisia annua* L using LC/MS/MS**; Huihua Ji[1]; Lowell Bush[1]; Neil Fannin[1]; [1]*University of Kentucky, Lexington, KY*

ThP 584 **Putative Identification of Phenolic Compounds and Evaluation of Antioxidant, Anti-Inflammatory and Neuroprotective Activities of Extracts of 3 Endemic Colombian Fruits**; Daniel Esteban Arias; *Professor, Bogota, Colombia*

ThP 585 **Using Dereplication for Targeted and Untargeted Re-Isolation of Fungal Secondary Metabolites**; Allison J. Wright[1]; Sonja L. Knowles[1]; Huzefa A. Raja[1]; Nicholas H. Oberlies[1]; [1]*University of North Carolina at Greensboro, Greensboro, NC*

ThP 586 **Screening of a Natural Product Library for Antimicrobial Activity Targeting Metal Homeostasis**; Charles Veltri[1]; Maria Lozoya[1]; Jennifer Foster[2]; Pete Manchen[2]; Cynthia Reck[3]; Genna Gallas[3]; Andrew Salywon[4]; Jose Hernandez[3]; [1]*Midwestern University College of Pharmacy-Glendale, Glendale, AZ;* [2]*Midwestern University Arizona College of Osteopathic Medicine, Glendale, AZ;* [3]*Midwestern University College of Graduate Studies-Glendale, Glendale, AZ;* [4]*Desert Botanical Garden, Phoenix, AZ*

ThP 587 **Uptake and Health Effects of Phytochemicals in Honey Bees and Their Larvae Investigated by LC-QTRAP-MS Quantitation and GC-TOF-MS Metabolomics**; Nanna H Vidkjaer[1]; Per Kryger[1]; Inge S Fomsgaard[1]; [1]*Aarhus University, Slagelse, Denmark*

ThP 588 **Enhancing Confidence in Screening and Quantitation of Phytochemicals in Herbal Extracts by Nominal Mass LC-MS/MS**; Prasanth Joseph[1]; Saikat Banerjee[1]; Samir Vyas[1]; [1]*Agilent Technologies, Whitefield, Bengaluru, India*

ThP 589 **Rapid Characterization of *Valeriana jatamansi* Jones Using Online Supercritical Fluid Extraction-High Performance Liquid Chromatography Combined with High Resolution Mass Spectrometry**; Jing Dong[1]; Shizhong Chen[2]; Naoki Hamada[1]; Xiaodong Li[1]; Satoshi Yamaki[1]; [1]*SHIMADZU CHINA MS CENTER, Beijing, China;* [2]*Peking University, Beijing, China*

NUCLEIC ACIDS AND OLIGONUCLEOTIDES II
590-611

ThP 590 **Determination of Length and Composition of polyA Tails in Phosphate-Modified *in vitro* Transcribed mRNAs using LC-MS/MS**; Dominika Strzelecka[1]; Miroslaw Smietanski[2]; Marcin Warminski[1]; Pawel Jan Sikorski[2]; Joanna Kowalska[1]; Jacek Jemielity[2]; [1]*Faculty of Physics, University of Warsaw, Warsaw, Poland;* [2]*Centre of New Technologies, University of Warsaw, Warsaw, Poland*

ThP 591 **The Effect of G-Quadruplexes on the Stability of Adjacent DNA Domains Studied by Temperature-Controlled nanoESI-MS**; Adam Pruška[1]; Adrien Marchand[1]; Renato Zenobi[1]; [1]*ETH Zurich, Zurich, Switzerland*

ThP 592 **Rapid Detection of Ribonucleoside Modifications by Liquid Chromatography Higher-Energy Collisional Dissociation Mass Spectrometry and Spectral Matching**; Manasses Jora[1]; Peter A. Lobue[1]; Robert L. Ross[1]; Balasubrahmanyam Addepalli[1]; Patrick A. Limbach[1]; [1]*Department of Chemistry, University of Cincinnati, Cincinnati, OH*

ThP 593 **Gas Phase Fractionation to Increase Sensitivity of a Data Dependent-Constant Neutral Loss-MS3(DDA-CNL/MS3) DNA Adductomic Analysis**; Valeria Guidolin[1]; Peter W. Villalta[2]; Foster Jacobs[2]; Silvia Balbo[1,2]; [1]*School of Public Health, University of Minnesota, Minneapolis, MN;* [2]*Masonic Cancer Center, Minneapolis, Minnesota*

ThP 594 **High Performance Oligonucleotide Analysis by HILIC-MS: Ion-Pairing Reagents Not Required**; Peter A. Lobue[1]; Manasses Jora[1]; Balasubrahmanyam Addepalli[1]; Patrick A. Limbach[1]; [1]*Department of Chemistry, University of Cincinnati, Cincinnati, OH*

ThP 595 **Construction of A New Porous Covalent Organic Polymer via Schiff-base Reaction and Its Application in Desalination of Oligonucleotides**; Li-Juan Wang[1,2]; Qian-Yu Zhou[1]; Yu-Fang Ma[1]; Yue Yu[1]; Ying-Lin Zhou[1]; Xin-Xiang Zhang[1]; [1]*Peking University, Beijing, China;* [2]*Hebei University, Baoding, China*

ThP 596 **LC-MS Detection of UV-Induced Oxidative Damage to Ribosomal RNA**; Mariana Bonafim Piveta[1]; Manasses Jora[1]; Patrick A Limbach[1]; Balasubrahmanyam Addepalli[1]; [1]*University of Cincinnati, Cincinnati, OH*

ThP 597 **Enzymatic Labeling of Oligonucleotides for Multiplexed LC-MS/MS**; Scott Abernathy[1]; Kayla M. Borland[2]; Peter A. Lobue[1]; Patrick A. Limbach[1]; [1]*University of Cincinnati, Cincinnati, OH;* [2]*Ludwig-Maximilians-University Munich, Munich, Germany*

ThP 598 **Improving Transfer RNA Isolation for more Accurate LC-MS/MS Characterization of Modified Nucleosides**; Ruoxia Zhao[1]; Robert L. Ross[1]; Andrew Wood[1]; Manasses Jora[1]; Patrick A Limbach[1]; [1]*University of Cincinnati, Cincinnati, OH*

ThP 599 **Development of High-Sensitive and High-Throughput Quantitative Analysis Method of Modified Nucleosides Using UHPLC-UniSpray /MS/MS**; Takahiro kogaki[1]; Ikumi Oshio[1]; Souta Iyama[1]; Hiroaki Hase[1]; Kentaro Jingushi[2]; Yuko Ueda[1]; Zenzaburo Tozuka[1]; Daisuke Saigusa[3]; Kazutake Tsujikawa[1]; [1]*Mol. Cell. Physiol., Grad. Sch. Pharm. Sci., Osaka University., Suita, Japan;* [2]*Department of Urological Immuno-oncology, Graduate School of Medicine, Osaka University, Suita, Japan;* [3]*Department of Integrative Genomics, Tohoku Medical Megabank Organization, Tohoku University, Sendai, Japan*

ThP 600 **Accurate Mass Determination of Long DNA Fragments Prepared for Structural Biology Study of Epigenetic DNA Methylation**; Hiroshi Ushijima[1]; Rena Maekawa[1]; Eri Igarashi[1]; Satoko Akashi[1]; [1]*Yokohama City University, Yokohama, Japan*

ThP 601 **A Software Platform for the Quality Control of Synthetic Oligonucleotides**; Detlev Suckau[1]; Sam Kyritsogiou[2]; Yue Ju[3]; Guillaume Tremintin[3]; Anjali Alving[4]; Michael Greig[3]; Robert Kane[3]; [1]*Bruker Daltonics, Bremen, Germany;* [2]*Kaneka Eurogentec SA, Liège, Belgium;* [3]*Bruker Scientific, San Jose, CA;* [4]*Bruker Daltonics Inc., Billerica, MA*

ThP 602 **Investigation of Matrix Conditions for Nucleic Acid Analysis in Positive Ion Detection Using a Linear Benchtop MALDI-TOFMS**; Shuichi Nakaya[1]; Akihiro Kunisawa[2]; Zenzaburo Tozuka[2]; Yuzo Yamazaki[1]; [1]*Shimadzu Corporation, Kyoto, Japan;* [2]*Shimadzu Analytical Innovation Research Laboratory, Osaka University, Suita, Japan*

ThP 603 **Pytheas: Software to Analyze and Map RNA Post-Transcriptional Modifications with Tandem MS and Stable Isotope Labelling**; Luigi D'Ascenzo, Ph.D. [1]; Anna Popova, Ph.D. [1]; James R. Williamson, Ph.D. [1]; [1]*The Scripps Research Institute, La Jolla, CA*

ThP 604 **Leveraging Ion-tagged Oligonucleotides and Mass Spectrometry for the Detection of RNA Modifications**; Kevin D. Clark[1]; Colin Lee[2]; Jonathan V. Sweedler[1,2];

[1]Beckman Institute, Urbana, IL; [2]University of Illinois at Urbana-Champaign, Urbana, IL

ThP 605 **Mass Spectrometry-Based Identification of Mono-Methylated RNA Nucleoside Positional Isomers: Application for Structural Analysis of RNA Modifications in the Leishmania ribosome**; Hiroshi Nakayama[1]; Yoshio Yamauchi[2]; Yuko Nobe[2]; Masami Koike[1]; Nobuhiro Takahashi[3]; Moran Shalev-Benami[4]; Toshiaki Isobe[2]; Masato Taoka[2]; *[1]RIKEN Center for Sustainable Resource Science, Wako, Japan; [2]Tokyo Metropolitan University, Hachioji, Japan; [3]Tokyo University of Agriculture and Technology, Fuchu, Japan; [4]Weizmann Institute of Science, Rehovot, Israel*

ThP 606 **High-throughput Oligonucleotide Analysis using RapidFire/TOF MS and OligoSearch Software**; Peter Rye[1]; Jim Lau[2]; Tony Brand[3]; *[1]Agilent Technologies, Lexington, MA; [2]Agilent Technologies, Wilmington, DE; [3]Agilent Technologies, Raleigh-Durham, NC*

ThP 607 **Simultaneous Quantification of dA-Ap and dG-Ap Interstrand Cross-Links in Cellular and Tissue DNA**; Su Guo[1]; Jiapeng Leng[1]; Yinsheng Wang[1]; *[1]UC Riverside, Riverside*

ThP 608 **Multiplex Quantification of RNA Methylation by Targeted Mass Spectrometry**; Jerome Vialaret[1]; Aurore Attina[1]; Helene Guillorit[2]; Amandine Bastide[2]; Sebastien Relier[2]; Jean Jacques Vasseur[3]; Francoise Debart[3]; Sylvain Lehmann[1]; ALexandre David[2]; Christophe Hirtz[1]; *[1]Montpellier University - LBPC/PPC, Montpellier, France; [2]Institut de Génomique Fonctionnelle, Montpellier, France; [3]Institut des Biomolécules Max Mousseron, Montpellier, France*

ThP 609 **Ultraviolet Photodissociation of Silver Nanocluster/ DNA Complexes**; Ines C Santos[1]; Molly S Blevins[1]; John Armstrong[1]; Christopher M Crittenden[1]; Jennifer S Brodbelt[2]; *[1]University of Texas at Austin, Department of Chemistry, Austin, TX; [2]The University of Texas, Austin, TX*

ThP 610 **MALDI MS Study of Activity of DNA Specific Enzymes in the Vicinity of G-Quadruplex Structures**; Alexandra V. Sekridova[1]; Galina E. Pozmogova[2]; Igor P. Smirnov[2]; *[1]Institute of agricultural biotechnology, Moscow, Russia; [2]Research and Clinical Center for Physical-Chemical Medicine, Moscow, Russia*

ThP 611 **Collision-Induced Dissociation Studies of protonated ions of Alkylated Thymidine and 2'-deoxyguanosine**; Yuxiang Cui[1]; Jun Yuan[1]; Pengcheng Wang[1]; Jun Wu[1]; Yang Yu[1]; Yinsheng Wang[1]; *[1]University of California, Riverside, Riverside, CA*

PEPTIDES: FRAGMENTATION MECHANISMS
612-617

ThP 612 **Metal Cationization of Immunopeptides for Improved Dissociation and Measurement by Differential Ion Mobility-Mass Spectrometry**; James E. Keating[1]; Chris Chung[1]; Shengjie Chai[2]; Benjamin G. Vincent[3]; Sally A. Hunsucker[3]; Paul M. Armistead[3]; Gary L. Glish[1]; *[1]Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC; [2]Curriculum in Genetics & Molecular Biology, University of North Carolina at Chapel Hill, Chapel Hill, NC; [3]Lineberger Comprehensive Cancer Center, University of North Carolina at Chapel Hill, Chapel Hill, NC*

ThP 613 **Investigation of CID and HCD Tandem Mass Spectra of Double Derivatized Histone (H3) Model Peptide Using High-Resolution Hybrid Mass Spectrometer**; Leila Afjehi-Sadat[1]; Benjamin A Garcia[1]; *[1]University of Pennsylvania, Philadelphia, PA*

ThP 614 **Comparative Study of Average Probabilities of Fragment Ion Formation in Peptides with Different Aspartate Isoforms**; Daniil Ivanov[1]; Stanislav Pekov[1,2]; Maria Indeykina[1,3]; Anna Bugrova[3]; Alexey Kononikhin[1,2,3]; Igor Popov[1,2]; Eugene (evgeny) Nikolaev[4]; *[1]Moscow Institute of Physics and Technology (State University), Dolgoprudny, Russia; [2]Institute for Energy Problems of Chemical Physics RAS, Moscow, Russia; [3]Institute of Biochemical Physics RAS, Moscow, Russia; [4]Skolkovo institute of science and technology, Moscow Region, Russian Federation*

ThP 615 **Combined Density Functional and Statistical Analyses of Doubly Protonated Tryptic Peptide Series**; Shanshan Guan[1]; Benjamin J Bythell[1]; *[1]University of Missouri, St. Louis, St. Louis, MO*

ThP 616 **Fast and Accurate MS² Peak Intensity Prediction for Multiple Fragmentation Methods, Instruments and Labeling Techniques**; Ralf Gabriels[1,2]; Lennart Martens[1,2]; Sven Degroeve[1,2]; *[1]VIB-UGent Center for Medical Biotechnology, Ghent, Belgium; [2]Department of Biomolecular Medicine, Ghent University, Ghent, Belgium*

ThP 617 **Optimizing Parallel HCD and ETD with supplemental HCD Data Acquisition using the Tribrid Oritrap Lumos**; Lauren R. DeVine[1]; Robert N. Cole[1]; *[1]Johns Hopkins University School of Medicine, Baltimore, MD*

PROTEINS: COMPLEXES/NON-COVALENT I NTERACTIONS II
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ThP 618 **Nanoscale Ion Emitters in Native Mass Spectrometry for Measuring Ligand-Protein Binding Affinities**; Giang Nguyen[1]; Thinh N. Tran[2]; Matthew N. Podgorski[3]; Stephen G. Bell[3]; Claudiu T. Supuran[4]; William A. Donald[1]; *[1]School of Chemistry, University of New South Wales, Sydney, NSW, Australia; [2]School of Electrical Engineering and Telecommunications, University of New South Wales, Sydney, NSW, Australia; [3]Department of Chemistry, University of Adelaide, Adelaide, Australia; [4]University of Florence, Department of Neuroscience, Psychology, Drug Research and Child's Health, Section of Pharmaceutical and Nutraceutical Sciences, Via Ugo Schiff 6, Sesto Fiorentino, Italy*

ThP 619 **Investigating the Interactions of the First 17 Residues of Huntingtin with Lipid Vesicles Using ESI-MS Experiments and MD Simulations.**; Ahmad Kiani Karanji[1]; Maryssa Beasely[1]; Ali Ranjbaran[2]; Justin Legleiter[1]; Stephen Valentine[1]; *[1]West Virginia University.C. Eugene Bennett Department of Chemistry, Morgantown, WV; [2]West Virginia University, Morgantown, WV*

ThP 620 **Intact Transition Epitope Mapping – Targeted High-Energy Rupture of Extracted Epitopes (ITEM - THREE)**; Bright D. Danquah[1]; Claudia Röwer[1]; Kwabena F.M. Opuni[2]; Reham A. El-Kased[3]; Harald Illges[4]; Cornelia Koy[1]; Michael O. Glocker[1]; *[1]Proteome Center Rostock, Rostock, Germany; [2]School of Pharmacy, University of Ghana, Legon, Ghana; [3]Microbiology and Immunology Faculty of Pharmacy, The British University in Egypt, Cairo, Egypt; [4]University of Applied Sciences Bonn-Rhein-Sieg, Bonn, Germany*

ThP 621 **The Application of Direct MS for the Investigation of Complex Biological Systems**; Gili Ben-Nissan[1]; Jelena Cvetichanin[1]; Ravit Netzer[1]; Sarel J Fleishman[1]; Michal Sharon[1]; *[1]Weizmann Institute of Science, Rehovot, Israel*

ThP 622 **Uniting Microchip Capillary Electrophoresis-MS and Ultraviolet Photodissociation Technologies for On-line Separation and Characterization of Native Protein Complexes**; M. Rachel Mehaffey[1]; Ashley Bell[2]; J. Scott Mellors[2]; Michael B. Lanzillotti[1]; Jennifer S. Brodbelt[1]; *[1]The University of Texas at Austin, Austin, TX; [2]908 Devices, Boston, MA*

ThP 623 **Native Ion-Mobility Mass Spectrometry of Staph. Aureus Alpha-Hemolysin Membrane Pore Complexes**; Jesse W Wilson[1]; Amber D Rolland[1]; Grant M Klausen[1]; Alexander S Skochko[1]; James S Prell[1]; *[1]University of Oregon Department of Chemistry and Biochemistry, Eugene, OR*

ThP 624 **Determination of Protein-Brain Ganglioside Interactions by Chip-Based Nanoelectrospray Quadrupole-Time-of-**

Flight Tandem Mass Spectrometry; Laurentiu Popescu[1]; Mirela Sarbu[1]; Raluca Ica[1]; Alina Petrut[1]; Alina D. Zamfir[2]; *[1]National Institute for Research and Development in Electrochemistry and Condensed Matter, Timisoara, Romania; [2]Nat'l Inst, Electrochemistry & Condensed Matter, Timisoara, Romania*

ThP 625 **High Resolution - Mass Spectrometry Cellular Thermal Shift Assay (HR-MS-CETSA)- Impact of Phosphorylation on Thermal Protein Stability**; Yan Ting Lim[1]; Tianyun Zhao[2]; Wint Wint Phoo[1]; Lingyun Dai[2]; Loo Chien Wang[1]; Liyan Chen[1]; Par Nordlund[1,2,3]; Radoslaw Sobota[1]; *[1]Institute of Molecular and Cell Biology Agency for Science, Technology and Research (A*STAR), Singapore, Singapore; [2]School of Biological Sciences, Nanyang Technological University, Singapore, Singapore, Singapore; [3]Karolinska Institutet, Department of Oncology-Pathology, Stockholm, Sweden*

ThP 626 **Data-Driven Detection of Functional Proteoforms in SEC-SWATH-MS Data**; Isabell Bludau[1]; Max Frank[1,2]; Moritz Heusel[1]; Yujia Cai[2]; George Rosenberger[3]; Yansheng Liu[4]; Ashok Venkitaraman[5]; Vihandha Wickramasinghe[6]; Ben C Collins[1]; Hannes Roest[2]; Ruedi Aebersold[1,7]; *[1]ETH Zurich, Zurich, Switzerland; [2]Donnelly Centre for Cellular and Biomolecular Research, University of Toronto, Toronto, ON; [3]Columbia University, New York, NY; [4]Yale University, New Haven; [5]Medical Research Council Cancer Unit, University of Cambridge, Cambridge, United Kingdom; [6]Peter MacCallum Cancer Centre, Melbourne, Australia; [7]University of Zurich, Zurich, Switzerland*

ThP 627 **Real-Time Enzymatic Catalysis by Variable-Temperature Nano-Electrospray Ionization Ion Mobility Spectrometry-Mass Spectrometry**; Brooke A. Brown[1]; Christopher R. Conant[1]; Tarick J. El-Baba[1]; Daniel W. Woodall[1]; David E. Clemmer[1]; *[1]Indiana University, Bloomington, IN*

ThP 628 **UVPD-MS of Protein-Ligand Complexes Governed by Different Binding Modes and Affinities**; Ines C Santos[1]; Jennifer S Brodbelt[1]; *[1]University of Texas at Austin, Austin, TX*

ThP 629 **Identifying Protein Complexes of Endocrine Disrupting Organotin Compounds Using Mild LC-MS Techniques**; Jonas M. Will[1]; Michael Sperling[1,2]; Uwe Karst[1]; *[1]University of Muenster, Institute of Inorganic and Analytical Chemistry, Muenster, Germany; [2]European Virtual Institute for Speciation Analysis (EVISA), Muenster, Germany*

ThP 630 **Investigation of Charge Partitioning from Gas-phase Dissociation of Dimeric Proteins**; Mengxuan Jia[1]; Chen Du[1]; Yang Song[1]; Zibo Chen[2]; David Baker[2]; Vicki H. Wysocki[1,3]; *[1]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, OH; [2]Department of Biochemistry, University of Washington, Seattle, WA; [3]Resource for Native Mass Spectrometry Guided Structural Biology, Columbus, OH*

ThP 631 **Identification of Smyd1's Chromatin Binding Partners via ChIP-MS**; Anna Bakhtina[1]; Aman Makaju[2]; Sarah Franklin[3]; *[1]University of Utah, Salt Lake City, UT; [2]University of Utah School of Medicine, Department of Biochemistry, Salt Lake City, Utah; [3]University of Utah School of Medicine, Salt Lake City, UT*

ThP 632 **High Resolution Structural Footprinting for 15-PGDH Inhibitor Binding Site Assessment**; Janna Kiselar[1]; Joseph Ready[2]; Yuan Yiyuan[1]; Mark R Chance[1]; Sanford Markowitz[1]; *[1]Case Western Reserve Univ, Cleveland, OH; [2]UT Southwestern, Dallas, TX*

ThP 633 **Integrated Structural Proteomics and Dynamics of a Solid-Body Organism by Combined XLMS, Solvent Accessible Surface Modification and QconCAT**; Yeya Mirzakhanyan[1]; Paul Gershon[1]; *[1]UC-Irvine, Irvine, CA*

ThP 634 **Analysis of Human Nuclear Protein Complexes by Quantitative Mass Spectrometry Profiling**; Katelyn E. Connelly[1]; Victoria Hedrick[2]; Tiago J. P. Sobreira[2]; Emily C. Dykhuizen, [1]; Uma K. Aryal[2]; *[1]Department of Medicinal Chemistry and Molecular Pharmacology Purdue University, West Lafayette, IN; [2]Purdue Proteomics Facility, Bindley Bioscience Center, West Lafayette, IN*

ThP 635 **Characterization of Protein-Ligand Binding Interactions of Polyphenol Inhibitors of FabI by Molecular Docking Simulations and Native MS**; P. Matthew Joyner[1]; Denise P. Tran[2]; Joseph A. Loo[2]; *[1]Pepperdine University, Malibu, CA; [2]UCLA, Los Angeles, CA*

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ThP 636 **Native Mass Spectrometry Analysis of Protein and Protein Complexes Formed from Non-volatile Salt Buffers through use of Gábor Transformation**; Sean P Cleary[1]; Jesse W Wilson[1]; James S Prell[1]; *[1]University of Oregon, Eugene*

ThP 637 **Integrated Structural Biology Study of Roundabout1 Interaction with Fondaparinux**; Robert Williams[1]; Jeong Yeh Yang[1]; Yunyun Gao[2]; Arwen Pearson[2]; Kelley Moremen[1]; James H. Prestegard[1]; I. Jonathan Amster[1]; *[1]University of Georgia, Athens, GA; [2]University of Hamburg, Hamburg, Germany*

ThP 638 **Unexpected Asp-isomerization Behavior in Monoclonal Antibodies: Connecting Primary Sequence with High Order Structure and Molecular Dynamics**; Andrew D Mahan[1]; Dorina Saro[1]; Jeffrey Brelsford[1]; Weiping Shen[1]; Sandeep Somani[1]; Hirsh Nanda[1]; *[1]Janssen R&D, Spring House, PA*

ThP 639 **Structural Characterization of Ternary Complexes for Selective Protein Degradation by Hydrogen-Deuterium Exchange Mass Spectrometry**; Jing Li[1]; Aaron Balog[1]; Louis Lombardo[1]; John Newitt[1]; Mark Witmer[1]; Guodong Chen[1]; *[1]Bristol-Myers Squibb, Princeton, NJ*

ThP 640 **Native Ion Mobility Mass Spectrometry as a Powerful Tool to Dissect α-Synuclein Conformational Space - Small Molecules, Metal Ions, PTMs**; Rani Moons[1]; Albert Konijnenberg[1]; Anne-Marie Lambeir[2]; Frank Sobott[1,3,4]; *[1]Biomolecular and Analytical Mass Spectrometry group, University of Antwerp, Belgium; [2]Laboratory of Medical Biochemistry, University of Antwerp, Belgium; [3]Astbury Centre for Structural Molecular Biology, University of Leeds, United Kingdom; [4]School of Molecular and Cellular Biology, University of Leeds, United Kingdom*

ThP 641 **Cytochrome c / Cardiolipin Interactions in Apoptosis: The Roles of Protein Auto-Oxidation and *in situ* Covalent Modifications**; Victor Yin[1]; Lars Konermann[2]; *[1]University of Western Ontario, London, ON; [2]University of Western Ontario, London , ON*

ThP 642 **Coupling FPOP with IM-MS for Detailed Structural Characterization of the Native Ensemble of cytochrome c**; Emily E Chea[1]; Daniel Deredge[1]; Lisa M Jones[1]; *[1]University of Maryland, Baltimore- School of Pharmacy, Baltimore, MD*

ThP 643 **Deep Profiling of Proteome Structural Changes by TMT-Mass Spectrometry**; Kaiwen Yu[1]; Junmin Peng[1]; *[1]St Jude Children's Research Hospital, Memphis, TN*

ThP 644 **Investigation of Gas-Phase Unfolding Transitions of Protein Ions Using Ion Mobility-Mass Spectrometry**; Micah T Donor[1]; Samantha O Shepherd[1]; James S Prell[1]; *[1]University of Oregon Department of Chemistry and Biochemistry, Eugene, OR*

ThP 645 **Metal-Induced Oxidation of Transthyretin Studied via Ion Mobility-Orbitrap Mass Spectrometry and Surface-Induced Dissociation**; Mehdi Shirzadeh[1]; Michael L Poltash[1]; Jacob W McCabe[1]; Klaudia I Kocurek[1]; zahra Moghadamchargari[1]; Arthur Laganowsky[1]; David H. Russell[1]; *[1]Texas A&M University, College Station, TX*

ThP 646 **Structural Analysis of Gas-Phase Phosphoproteins;** Carter Lantz[1]; Rachel R. Ogorzalek Loo[1]; Joseph A. Loo[1]; *[1]University of California Los Angeles, Los Angeles, CA*

ThP 647 **Protein Structural Accessibility Differences in Cerebrospinal Fluid by Limited Proteolysis-Mass Spectrometry;** Danielle A Faivre[1]; Eric L Huang[1]; Michael J MacCoss[1]; *[1]University of Washington, Seattle, WA*

ThP 648 **Assessing the Comparability of Ion Mobility Mass Spectrometry to Measure Collision Cross Section Distributions for Protein Standards;** Aidan P France[1]; Lukasz Migas[2]; Bruno Bellina[2]; Eleanor Sinclair[2]; Perdita E. Barran[2]; *[1]University of Manchester, Manchester, United Kingdom; [2]Manchester Institute of Biotechnology, University of Manchester, United Kingdom*

ThP 649 **Distinguishing Subtle Conformational Differences in Protein Complexes using Ion Mobility Mass Spectrometry and Collision Induced Unfolding;** Stacey Nash[1]; Tyler Marcinko[1]; Richard W. Vachet[1]; *[1]University of Massachusetts at Amherst, Amherst, MA*

ThP 650 **MALDI Analysis for Protein Footprinting;** Jerry Jiang[1]; Michael L Gross[1]; Nicole D Wagner[1]; *[1]Washington University in St. Louis, St. Louis*

ThP 651 **Characterization and Biochemical Analysis of a Low-Molecular Weight Cysteine-Rich Protein in Black Widow Dragline Silk;** Mikayla Shanafelt[1]; Jared Deyarmin[1]; Ryan Hekman[2]; Taylor Rabara[1]; Camille Larracas[3]; Liang Xue[1]; Craig Vierra[1]; *[1]University of the Pacific, Stockton, CA; [2]Boston University, Boston, MA; [3]University of the Pacific, San Francisco, CA*

ThP 652 **Characterization of Co-Existing Enfuvirtide Conformational States by Ion Mobility Mass Spectrometry and Hydrogen/Deuterium Exchange;** Bradley Stocks[1]; Gregory H. Bird[2]; Loren D. Walensky[2]; Jeremy E. Melanson[1]; *[1]National Research Council Canada, Ottawa, ON; [2]Dana-Farber Cancer Institute, Boston, MA*

ThP 653 **Microcontoller Timing, OPO and FPOP for T-Jump Measurement of Protein Conformational Kinetics;** Don L Rempel[1]; Roger (Xiaoran) Liu[2]; Michael L Gross[2]; *[1]Washington University, St Louis, MO; [2]Washington University, St.louis, MO*

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ThP 654 **Better Investigation of Integrin Expression in Cancer Cell Lines by Comparison of Different Membrane Protein Enrichment Methods;** Mona Goli[1]; Jair Montford[1]; Katya Y Torres-Ulloa[1]; Wenjing Peng[1]; Ahmed Hussien[1,2]; Yehia Mechref[1]; *[1]Texas Tech University, Lubbock, TX; [2]University of Alexandria, Alexandria, Egypt*

ThP 655 **Co-Localization of CD147 with Oncogenic Proteins Confers Drug-Resistant Phenotype in Breast Cancer Stem Cells;** Sohyun Kim[1]; Yuri Seo[1]; Hyeryeon Jung[1]; Jieun Jung[2]; Yeojin Jung[2]; Kristine M Kim[2]; Eugene C Yi[1]; *[1]Department of Molecular Medicine and Biopharmaceutical Sciences, Graduate School of Convergence Science and Technology, Seoul National University, Seoul, South Korea; [2]College of Biomedical Science, Kangwon National University, Seoul, South Korea*

ThP 656 **Novel Strategies for Top-down Proteomics of Endogenous Membrane Protein Complexes;** Kyle Brown[1]; Bifan Chen[1]; Ziqing Lin[1]; Tania Guardado[1]; Song Jin[1]; Ying Ge[1]; *[1]University of Wisconsin-Madison, Madison, WI*

ThP 657 **Comparative Proteomic Profiling of Five 2D and 3D Grown Cancer Cell Lines Using HRAM LC-MS.;** Josip Blonder[1]; Jan A Kaczmarczyk[1]; Rhonda R Roberts[1]; Gordon R Whiteley[1]; Robin A Felder[2]; Richard G Saul[1]; *[1]Frederick Nat'l Lab for Cancer Research, Frederick,MD; [2]Department of Pathology, University of Virginia School of Medicine, Charlottesville, VA*

ThP 658 **Evaluation of Six Different Sample Preparation Strategies for Enhanced In-Depth Proteomic Analysis of Milk Fat Globule Membrane;** Yongxin Yang[1]; Ruchika Bhawal[2]; Elizabeth T. Anderson[2]; Sheng Zhang[2]; *[1]Anhui Academy of Agricultural Sciences, Hefei Shi, China; [2]Cornell University, Ithaca, NY.*

ThP 659 **Selective Binding of a Toxin and Phosphatidylinositides to a Mammalian Potassium Channel;** Yang Liu[1]; Michael L Poltash[2]; Wen Liu[1]; David H. Russell[2]; Arthur Laganowsky[2]; *[1]TAMU Health Science Center, Houston, TX; [2]Texas A&M University, College Station, TX*

ThP 660 **Quantification of Mitochondrial Membrane Proteins in Dried Blood Spots for the Detection of Blood Doping Practices in Sport;** Holly Cox[1]; Abhilasha Manandhar[1]; Daniel Eichner[1]; *[1]Sports Medicine Research and Testing Laboratory, Salt Lake City, UT*

ThP 661 **Native MS and Surface Induced Dissociation Provide Insight into Eye Lens Aquaporins;** Sophie R Harvey[1,2]; Wendy L White[3]; Zachary L VanAernum[1,2]; Erin M Panczyk[1,2]; Kevin L Schey[3]; Vicki H Wysocki[1,2]; *[1]Department of Chemistry and Biochemistry, The Ohio State University, Columbus, Ohio; [2]Resource for Native Mass Spectrometry Guided Structural Biology, The Ohio State University, Columbus, Ohio; [3]Department of Biochemistry, Vanderbilt University, Nashville, Tennessee*

ThP 662 **Detergents' Supercharging Effects on Soluble Proteins and Membrane Proteins;** Wonhyeuk Jung[1]; Frederik Lermyte[2]; Carter Lantz[1]; Rachel Loo[1]; Joseph A. Loo[1]; *[1]UCLA, Los Angeles, CA; [2]University Of Antwerp, Antwerp, Belgium*

ThP 663 **Intact and Subunit Mass Analysis Using Native Ion Exchange Chromatography Coupled to an Orbitrap Mass Spectrometer;** Qian Liu[1]; Stephane Houel[1]; Hao Zhang[1]; Alla Polozova[1]; *[1]Amgen Inc., Cambridge, MA*

ThP 664 **Proteomic Analysis of Cell Surface Proteins with Improved Specificity of Enrichment;** Betsy Benton[1]; Sergei Snovida[1]; Katherine Herting[1]; Hongbin Zhu[1]; John C. Rogers[1]; Barbara Kaboord[1]; *[1]Thermo Fisher Scientific, Rockford, IL*

ThP 665 **Probing Adhesion GPCR-G Protein Interaction by Chemical Cross-Linking and Mass Spectrometry;** Bill Huang[1]; Hee-Yong Kim[1]; *[1]NIAAA/NIH, Rockville, MD*

ThP 666 **Applying a Quantitative, Cell Surface Glycoproteomic Approach to Understanding Phenotypic Changes Induced by Extended Culturing of Explanted Human Cardiac Fibroblasts;** Linda Berg Luecke[1]; Amanda Rae Buchberger[1,2]; Matthew Waas[1]; Rebekah L. Gundry[1,2]; *[1]Medical College of Wisconsin, Milwaukee, WI; [2]Center for Biomedical Mass Spectrometry Research, Medical College of Wisconsin, Milwaukee, WI*

ThP 667 **Ion Mobility-Mass Spectrometry Reveals α-Synuclein Conformational Changes within Lipid Bicelles;** Denise P Tran[1]; Joseph A Loo[1]; *[1]UCLA, Los Angeles, CA*

ThP 668 **Application of the CellSurfer Platform Enables Generation of a Chamber-Resolved Map of Surface N-Glycoproteins on Primary Human Cardiomyocytes;** Rachel A. Jones Lipinski[1]; Ranjuna Weerasekera[1]; Linda Berg Luecke[1]; Amanda Rae Buchberger[1]; Matthew Waas[1]; Rebekah L. Gundry[1]; *[1]Medical College of Wisconsin, Milwaukee, WI*

ThP 669 **Comparison of Reverse Phase and Ion Exchange Fractionation Strategies for 2D-LC-MS/MS Based Liver Proteomics;** Maxime Sansoucy[1]; Felix Friedrich[1]; Lekha Sleno[1]; *[1]UQAM, Montreal, QC*

ThP 670 **Characterization of the Intact Proteins of Influenza Primary Liquid Standards;** Lidoshka Marc[1]; John R Barr[1]; Tracie Williams[1]; *[1]Centers for Disease Control and Prevention, Atlanta, Georgia*

ThP 671 **Bioinformatic Analysis of MS Data to Assess G-Protein Coupled Receptor Targets for Transactivation of**

Proliferative Pathways in Cancer Cells; Arba Karcini[1]; Iulia M. Lazar[1]; *[1]Virginia Tech, Blacksburg, VA*

ThP 672 **Therapeutic Utility of LIFR Inhibitor EC359 in Treating HDAC Inhibitor Resistance in Ovarian Cancer**; Suryavathi Viswanadhapalli[1]; Susan T. Weintraub[1]; Mengxing Li[1]; Hareesh B. Nair[2]; Klaus J. Nickisch[2]; Sammy Pardo[1]; Dana Molleur[1]; Ratna K. Vadlamudi[1]; *[1]University of Texas Health Science Center at San Antonio, San Antonio, TX; [2]Evestra, San Antonio, TX*

ThP 673 **LC-MS Characterization of Polysorbate 80 Raw Materials from Multi-Use Containers**; Rashmi Menon[1]; Erin Laskowich[1]; Linda Yi[1]; *[1]Biogen, Morrisville, NC*

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ThP 674 **Developing Novel Enrichment Strategies to Facilitate Proteomic Analysis of NR5A2in Triple Negative Breast Cancer**; Valentine V Courouble[1]; Yuanjun He[1]; Ruben Garcia-Ordonez[1]; Patrick R. Griffin[1]; *[1]Scripps Research, Jupiter, FL*

ThP 675 **Surface Glycoproteomic Analysis Reveals that Both Unique and Differential Expression of Surface Glycoproteins Determine the Cell Type**; Suttipong Suttapitugsakul[1]; Lindsey D. Ulmer[1]; Chendi Jiang[1]; Fangxu Sun[1]; Ronghu Wu[1]; *[1]Georgia Institute of Technology, Atlanta, GA*

ThP 676 **Proteomic Differences and Protein Acetylation by Sirtuins in Response to Cell Aging**; Liting Deng[1]; Mehdi Mirzaei[1]; Paul Andrew Haynes[1]; *[1]Macquarie University, Sydney, Australia*

ThP 677 **PPPome Profiling Using Quantitative Proteomics Reveals the Role of PP2Ac phosphorylation in Regulating PP2A-B55 Mediated Dephosphorylation of Mitotic Substrates**; Isha Nasa[1,2]; Lauren Cressey[1]; Thomas Kruse[3]; Emil PT Hertz[3]; Jakob Nilsson[3]; Arminja N Kettenbach[1,2]; *[1]Department of Biochemistry and Cell Biology, Dartmouth College, Hanover, NH; [2]Norris Cotton Cancer Center, Lebanon, NH; [3]Novo Nordisk A/S, Måløv, Denmark*

ThP 678 **Improving Confidence and Productivity for N-Linked Glycan Analysis in Biotherapeutics Development Using an Integrated and Compact LC-FLR-HRMS System**; Ximo Zhang[1]; Corey Reed[1]; Henry Shion[1]; Robert Birdsall[1]; Ying Qing Yu[1]; *[1]Waters Corporation, Milford, MA*

ThP 679 **Phosphonate-Modified Core-Shell Structured Fe3O4-SiO2 Nanoparticles: Synthesis, Characterization and Application to the Enrichment of Phosphopeptides**; Qingshi Meng[1]; Xiaohui Feng[1]; Xiangfang Tang[1]; Hongfu Zhang[1]; *[1]Institute of Animal Sciences, CAAS, Beijing, China*

ThP 680 **The Acetylation of Lysine-376 of G3BP1 Regulates RNA Binding and Stress Granule Dynamics**; Jing Chen[1]; Jozsef Gal[2]; Duck-Young Na[2]; Laura Tichacek[2]; Kelly R Barnett[2]; Haining Zhu[2,3]; *[1]University of Kentucky, Lexington, KY; [2]University of Kentucky, Lexington, Kentucky; [3]Lexington VA Medical Center, Research & Development, Lexington, Kentucky*

ThP 681 **Ischemic Stress to Kidneys from SIRT5 Mice is mitigated by Succinylation Response**; Kevin Peasley[1]; Anja N Holtz[2]; Nathan Basisty[2]; Takuto Chiba[1]; Birgit Schilling[2]; Sunder Sims-Lucas[1]; Eric Goetzman[1]; *[1]University of Pittsburgh, Pittsburgh, PA; [2]Buck Institute, Novato, CA*

ThP 682 **Middle-Down Characterization of Poly-Ubiquitin by 193 nm UVPD and EThcD**; Aarti Bashyal[1]; Jennifer S Brodbelt[1]; *[1]University of Texas - Austin, Austin, TX*

ThP 683 **LC-MS Analysis of Bound Sulfane Sulfur in Hypoxic Endothelial Cells**; Xinggui Shen[1]; Christopher B. Pattillo B. Pattillo[1]; Hyung W. Nam[1]; Christopher G. Kevil[1]; *[1]LSU Health-shreveport, Shreveport, LA*

ThP 684 **Ion-Exchange Chromatography On-Line Hyphenated to Mass Spectrometry for the Native Intact In-Depth Characterisation of Cationic and Anionic Proteins**; Florian Fuessl[1]; Angela Criscuolo[2]; Ken Cook[3]; Jonathan Bones[1]; *[1]Nibrt, Dublin, Ireland; [2]Institute of Bioanalytical Chemistry, Faculty of Chemistry and Mineralogy, Leipzig, Germany; [3]Thermo Fisher Scientific, Hemel Hempstead, UK, Hemel Hempstead, United Kingdom*

ThP 685 **Proteome-Wide Detection of Cysteine Nitrosylation Targets and Motifs Using Bioorthogonal Cleavable-Linker-Based Enrichment and Switch Technique (Cys-BOOST)**; Ruzanna Mnatsakanyan[1]; Stavroula Markoutsa[1]; Steven H.L. Verhelst[1,2]; René Zahedi[3]; *[1]Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Dortmund, Germany; [2]Laboratory of Chemical Biology, Department of Cellular and Molecular Medicine, KU Leuven - University of Leuven, Leuven, Belgium; [3]Segal Cancer Proteomics Centre, Lady Davis Institute for Medical Research, Jewish General Hospital, McGill University, Montreal, QC*

ThP 686 **Quantitative Middle Down Proteomics of Histone H3 Variant-Specific Proteoforms**; Tao Wang[1]; Matthew V. Holt[1]; Nicolas L. Young[1]; *[1]Baylor College of Medicine, Houston, TX*

ThP 687 **Analysis of the Human Brain Ubiquitylation Pattern Associated with Alzheimer's Disease Using Quantitative Proteomics**; Measho Abreha[1]; Eric B. Dammer[1,2]; Lingyan Ping[1,2]; Tian Zhang[1]; Duc M Duong[1,3]; Maria Gearing[1]; James J. Lah[1]; Allan I. Levey[1]; Nicholas T. Seyfried[1,2]; *[1]Emory University - Center of Neurodegenerative Diseases, Atlanta, GA; [2]Emory University-Biochemistry, Atlanta, GA; [3]Emory Integrated Proteomics Core, Emory University, Atlanta, GA*

ThP 688 **System-Wide Temporal Characterization of the Phosphoproteome of esophageal squamous Cell Carcinoma Cells**; Jun Adachi; *National Institutes of Biomedical Innovation, Health and Nutrition, Ibaraki, Japan*

ThP 689 **Scop3P: The Bridge between Human Phosphosites, Protein Structure and Proteomics Data**; Pathmanaban Ramasamy[1,2,3,4]; Demet Turan[1,2]; Elien Vandermarliere[1,2]; Lennart Martens[1,2]; Wim Vranken[3,4]; *[1]VIB-UGent Center for Medical Biotechnology, Ghent, Belgium, Gent, Belgium; [2]Department of Biochemistry, Faculty of Health Sciences, Ghent University, Ghent, Belgium, Gent, Belgium; [3]Interuniversity Institute of Bioinformatics in Brussels, ULB-VUB, Brussels, Belgium; [4]Structural Biology Brussels, Vrije Universiteit Brussel, Brussels, Belgium*

ThP 690 **Sequence Liability and Developability Assessment of mAb-A**; Samuel Korman[1]; Mingyan Cao[2]; Dengfeng Liu[2]; Sri Hari Raju Mulagapati[2]; *[1]Medimmune, Gaithersburg, MD; [2]MedImmune, Gaithersburg, MD*

ThP 691 **Cross-talk between Crucial Protein Post-Translational Modifications (PTMs): O-GlcNAcylation, Phosphorylation, and lys-acetylation**; Junfeng Ma; *Georgetown Univ., Washington, DC*

ThP 692 **Ubiquitinome Dynamics Upon Proteasome Modulation**; Jeroen Demmers; *Erasmus University Medical Center, Rotterdam, Netherlands*

ThP 693 **Exploring the Open Proteome: Proteomics Open Search Analysis with PTM-Shepherd**; Daniel J Geiszler[1]; Andy T. Kong[1]; Dmitry M Avtonomov[1]; Felipe Da Veiga Leprevost[1]; Hui-Yin Chang[1]; Alexey I. Nesvizhskii[1]; *[1]University of Michigan, Ann Arbor, MI*

ThP 694 **Investigation of KRAS 4B C-terminal peptides**; James Wilkins; *UCSF, San Francisco, CA*

ThP 695 **Impact of Oxidants on Anastellin - a Mediator of Fibronectin Assembly**; Per Hägglund[1]; Jianfei He[2]; Huan Cai[2]; Eva Ramos Becares[2]; Pontus Gourdon[2]; Michael J Davies[2]; *[1]University of Copenhagen, Copenhagen N, Denmark; [2]University of Copenhagen, Copenhagen, Denmark*

ThP 696 **Identification and Functional Characterizations of Novel Proteins Promoting α-N-demethylation**; David Bade[1];

Lin Li[1]; Xiaoxia Dai[1]; Yinsheng Wang[1]; [1]*UC Riverside, Riverside, CA*

ThP 697 **Streamlined Workflows for N-Glycan Analysis of Biotherapeutics Using InstantPC and 2-AB with LC-FLD-MS**; John Yan[1]; Andres Guerrero[1]; Ace G Galermo[1]; Ted Haxo[1]; Sergey Vlasenko[1]; Justin Hyche[1]; Tom Rice[1]; Aled Jones[1]; [1]*ProZyme, A part of Agilent, Hayward, CA*

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ThP 698 **Treasure Hunt for Peptides with Undefined Chemical Modifications: Revealing Differential Albumin Adducts of 2-Nitroimidazole-Indocyanine Green in Hypoxic Tumors**; Lei Wang[1]; Christopher Dietz[1]; Feifei Zhou[2]; Mohsen Erfanzadeh[2]; Quing Zhu[2,3]; Michael Smith[1]; Xudong Yao[1]; [1]*Department of Chemistry, University of Connecticut, Storrs, CT;* [2]*Department of Electrical and Computer Engineering, University of Connecticut, Storrs, CT;* [3]*Department of Biomedical Engineering, Washington University, St. Louis, MO*

ThP 699 **A Proline/Alanine-Specific Protease for Bottom-up Mass Spectrometry Workflows**; Chris Hosfield[1]; Michael Rosenblatt[1]; Marjeta Urh[1]; [1]*Promega, Madison, WI*

ThP 700 **Cysteine-Selective Middle-Down Proteomics with Ultraviolet Photodissociation Analysis**; Sean D Dunham[1]; Jennifer S Brodbelt[1]; [1]*University of Texas at Austin, Austin, TX*

ThP 701 **Carrier-Assisted Single-Tube Processing Approach for Targeted Proteomics Analysis of Low Numbers of Mammalian Cells**; Pengfei Zhang[1]; Matthew J. Gaffrey[1]; Ying Zhu[1]; William B. Chrisler[1]; Thomas L Fillmore[1]; Carrie D. Nicora[1]; Wei-Jun Qian[1]; Richard D. Smith[1]; Tao Liu[1]; Tujin Shi[1]; [1]*PNNL, Richland, WA*

ThP 702 **Enhancing Middle-Down Proteomics by Limited Carbamylation of Intact Proteins and Lys-C Digestion**; Michael B Lanzillotti[1]; Jennifer S Brodbelt[1]; [1]*University of Texas at Austin, Austin, TX*

ThP 703 **An MS Approach based on Randomized Phospho-peptide Libraries to Study the Sequence Preference of Protein Phosphatases 1 and 2A**; Bernhard Hoermann[1,2]; Dominic Helm[3]; Thomas Kokot[1]; Jeremy Chojnacki[1]; Mikhail Savitski[2,3]; Maja Koehn[1,2]; [1]*BIOSS Centre for Biological Signaling, Freiburg University, Freiburg, Germany;* [2]*Genome Biology Unit, EMBL, Heidelberg, Germany;* [3]*Proteomics Core Facility, EMBL, Heidelberg, Germany*

ThP 704 **A Novel Automated LC-MS Data Processing Platform for Immuno Reactivity Assessment of Antibodies Developed against Host Cell Proteins**; Yu Zhou[1]; Meghna Patel[1]; Riccardo Staccini[1]; Geuncheol Gil[1]; Sushmita Mimi Roy[1]; [1]*BioMarin, Novato, CA*

ThP 705 **Systematic Identification of Direct Substrates of Src Homology 2 Containing Protein Tyrosine Phosphatase 2**; Peipei Zhu[1]; Ruoyu Zhang[2]; Chuan-Chih Hsu[3]; Zhong-Yin Zhang[2]; Weiguo Andy Tao[2]; [1]*Purdue University, West Lafayette, IN;* [2]*Purdue University, West Lafayette, IN;* [3]*Stanford University, Stanford, CA*

ThP 706 **Assessing Protein Sequence Database Suitability Using *de novo* Sequencing**; Richard S. Johnson[1]; Brook L. Nunn[1]; Brian C Searle[2,3]; Molly Phillips[1,4]; Chris T. Amemiya[4]; Michelle Heck[5]; Micheal J MacCoss[1]; [1]*University of Washington, Seattle, WA;* [2]*Institute for Systems Biology, Seattle, WA;* [3]*Proteome Software, Portland, OR;* [4]*University of California, Merced, Merced, CA;* [5]*USDA ARS, Ithaca, NY*

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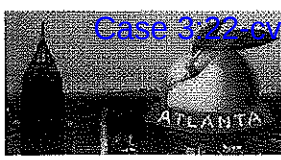
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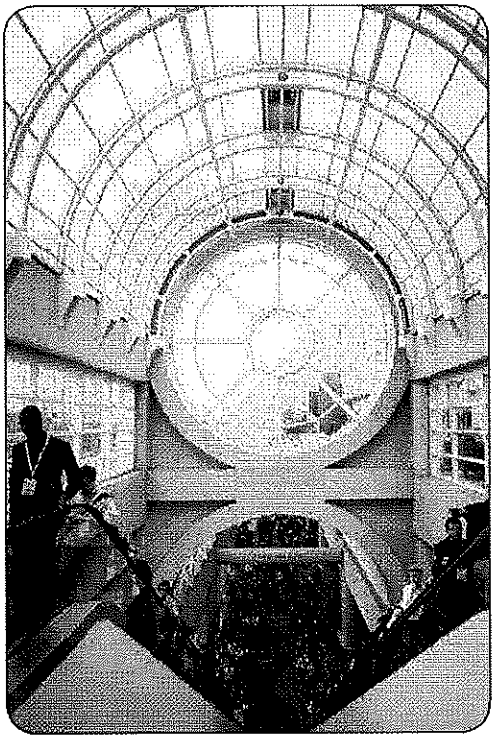
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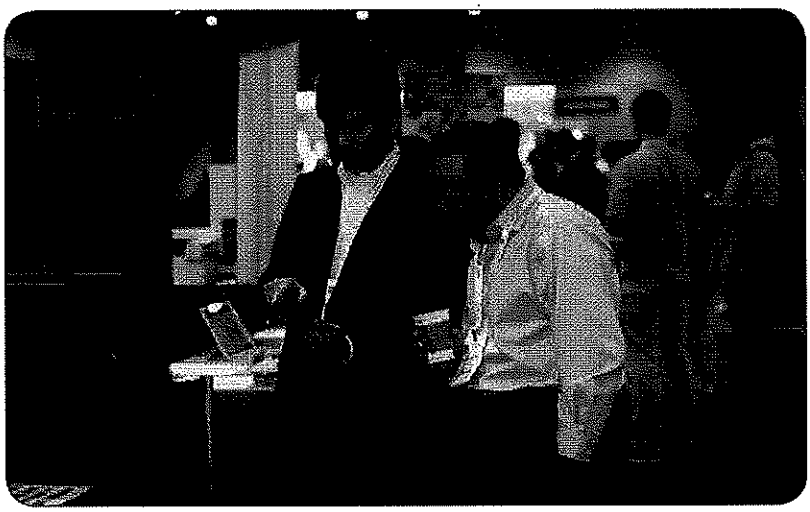
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